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L3             50 SEA SSS SAM L2
L4           3536 SEA SSS FUL L2
                  SAVE L4 DAVIS494/A TEMP

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     FILE 'REGISTRY' ENTERED AT 15:05:45 ON 17 OCT 2006

     FILE 'STNGUIDE' ENTERED AT 15:05:48 ON 17 OCT 2006

     FILE 'REGISTRY' ENTERED AT 15:07:42 ON 17 OCT 2006
L6                STRUCTURE UPLOADED
                  D QUE L6
L7             0 SEA SUB=L4 SSS SAM L6
L8             2 SEA SUB=L4 SSS FUL L6
                  D SCAN

     FILE 'HCAPLUS' ENTERED AT 15:08:55 ON 17 OCT 2006
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L17           29 SEA SUB=L4 SSS SAM L16
L18          743 SEA SUB=L4 SSS FUL L16
                  SAVE L18 DAVIS494SUB/A TEMP

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L21           36 SEA ABB=ON  PLU=ON  (L19 OR L1)
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                OR "BRIDGER GARY JAMES"/AU)
                E MCEACHERN E/AU
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L24          68 SEA ABB=ON  PLU=ON  ("SKERLJ R"/AU OR "SKERLJ R T"/AU OR
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L25         205 SEA ABB=ON  PLU=ON  ("SCHOLS D"/AU OR "SCHOLS DOMINIQUE"/AU OR
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L36          34 SEA ABB=ON  PLU=ON  L19 NOT L32

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FILE COVERS 1907 - 17 Oct 2006  VOL 145 ISS 17
FILE LAST UPDATED: 15 Oct 2006  (20061015/ED)

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J"/AU OR "BRIDGER G L"/AU OR "BRIDGER G M"/AU OR "BRIDGER G P"/AU OR "BRIDGER G W"/AU OR "BRIDGER GARY"/AU OR "BRIDGER GARY J"/AU OR "BRIDGER GARY JAMES"/AU)

L23 27 SEA FILE=HCAPLUS ABB=ON PLU=ON ("MCEACHERN E"/AU OR "MCEACHER N E J"/AU OR "MCEACHERN ERNEST"/AU OR "MCEACHERN ERNEST J"/AU OR "MCEACHERN ERNEST JOHN"/AU OR "MCEACHERN ERNIE J"/AU)

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L29 19 SEA FILE=HCAPLUS ABB=ON PLU=ON L24 AND L25

L30 23 SEA FILE=HCAPLUS ABB=ON PLU=ON (L27 AND (L28 OR L29)) OR (L28 AND L29)

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L32 38 SEA FILE=HCAPLUS ABB=ON PLU=ON (L31 OR L30)

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L32 ANSWER 1 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:1313985 HCAPLUS Full-text

DOCUMENT NUMBER: 144:51456

TITLE: Preparation of acylaminoalkylpiperidinamines as CCR5 ***chemokine*** receptor ligands

INVENTOR(S): Zhou, Yuanxi; ***Bridger, Gary J.***; ***Skerlj, Renato T.***; Bogucki, David; Yang, Wen; Bourque, Elyse; Langille, Jonathan; Li, Tong-Shuang; Metz, Markus

PATENT ASSIGNEE(S): Anormed Inc., Can.

SOURCE: U.S. Pat. Appl. Publ., 83 pp., Cont.-in-part of U.S. Ser. No. 12,002.
CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2005277668	A1	20051215	US 2005-152589		20050614
US 2005277670	A1	20051215	US 2004-12002		20041213
PRIORITY APPLN. INFO.:			US 2003-528975P	P	20031211
			US 2004-12002	A2	20041213

OTHER SOURCE(S): MARPAT 144:51456

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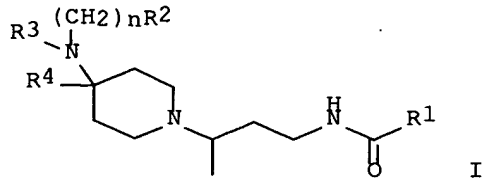

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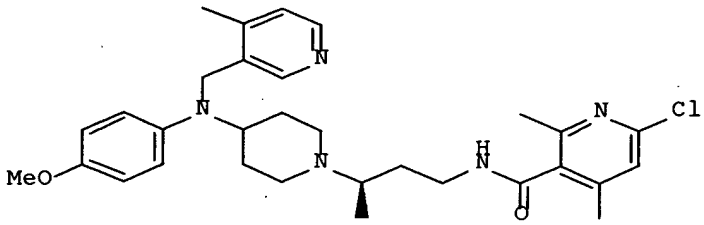

II

AB Title compds. [I; R1 = (substituted) aryl, heteroaryl; R2 = (substituted) pyridyl; R3 = (substituted) aryl, heteroaryl, cycloalka-fused Ph; R4 = H, alkyl; n = 0, 1], were prepared Thus, [1-[(R)-3-amino-1-methylpropyl]piperidin-4-yl](4-methoxyphenyl)(4-methylpyridin-3-ylmethyl)amine, 6-chloro-2,4-dimethylnicotinic acid, HOBT, EDCI, and diisopropylethylamine were stirred together in DMF overnight to give 80% title compound (II). Many I inhibited HIV-1 in vitro with IC50's in the range 0.01 nM to 50 μM.

L32 ANSWER 2 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:1214996 HCAPLUS Full-text
DOCUMENT NUMBER: 144:106405
TITLE: Pro-inflammatory properties of stromal cell-derived factor-1 (CXCL12) in collagen-induced arthritis
AUTHOR(S): De Klerck, Bert; Geboes, Lies; Hatse, Sigrid; Kelchtermans, Hilde; Meyvis, Yves; Vermeire, Kurt; ***Bridger, Gary***; Billiau, Alfons; ***Schols, Dominique***; Matthys, Patrick
CORPORATE SOURCE: Laboratory of Immunobiology, Rega Institute, Katholieke Universiteit Leuven, Louvain, Belg.
SOURCE: Arthritis Research & Therapy (2005), 7(6), R1208-R1220
CODEN: ARTRCV; ISSN: 1478-6362
URL: http://arthritis-research.com/content/pdf/ar1806.pdf
PUBLISHER: BioMed Central Ltd.
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: English

AB CXCL12 (stromal cell-derived factor 1) is a unique biol. ligand for the ***chemokine*** receptor CXCR4. We previously reported that treatment with a specific CXCR4 antagonist, AMD3100, exerts a beneficial effect on the development of collagen-induced arthritis (CIA) in the highly susceptible IFN-γ receptor-deficient (IFN-γR KO) mouse. We concluded that CXCL12 plays a central role in the pathogenesis of CIA in IFN-γR KO mice by promoting delayed type hypersensitivity against the auto-antigen and by interfering with chemotaxis of CXCR4+ cells to the inflamed joints. Here, we investigated whether AMD3100 can likewise inhibit CIA in wild-type mice and analyzed the

underlying mechanism. Parenteral treatment with the drug at the time of onset of arthritis reduced disease incidence and modestly inhibited severity in affected mice. This beneficial effect was associated with reduced serum concns. of IL-6. AMD3100 did not affect anti-collagen type II antibodies and, in contrast with its action in IFN-γR KO mice, did not inhibit the delayed type hypersensitivity response against collagen type II, suggesting that the beneficial effect cannot be explained by inhibition of humoral or cellular autoimmune responses. AMD3100 inhibited the in vitro chemotactic effect of CXCL12 on splenocytes, as well as in vivo leukocyte infiltration in CXCL12-containing s.c. air pouches. We also demonstrate that, in addition to its effect on cell infiltration, CXCL12 potentiates receptor activator of NF-κB ligand-induced osteoclast differentiation from splenocytes and increases the calcium phosphate-resorbing capacity of these osteoclasts, both processes being potently counteracted by AMD3100. Our observations indicate that CXCL12 acts as a pro-inflammatory factor in the pathogenesis of autoimmune arthritis by attracting inflammatory cells to joints and by stimulating the differentiation and activation of osteoclasts.

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 3 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:690115 HCAPLUS Full-text
DOCUMENT NUMBER: 143:205830
TITLE: AMD3465, a monomacrocyclic CXCR4 antagonist and potent HIV entry inhibitor
AUTHOR(S): Hatse, Sigrid; Princen, Katrien; De Clercq, Erik; Rosenkilde, Mette M.; Schwartz, Thue W.; Hernandez-Abad, Pedro E.; ***Skerlj, Renato T.***; ***Bridger, Gary J.***; ***Schols, Dominique***
CORPORATE SOURCE: Laboratory of Virology and Chemotherapy, Rega Institute for Medical Research, Katholieke Universiteit Leuven, Louvain, B-3000, Belg.
SOURCE: Biochemical Pharmacology (2005), 70(5), 752-761
CODEN: BCPCA6; ISSN: 0006-2952
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The ***chemokine*** receptors CCR5 and CXCR4 function as coreceptors for human immunodeficiency virus (HIV) and are attractive targets for the development of anti-HIV drugs. The most potent CXCR4 antagonists described until today are the bicyclams. The prototype compound, AMD3100, exhibits potent and selective anti-HIV activity against CXCR4-using (X4) viruses and showed antiviral efficacy in X4 HIV-1-infected persons in a phase II clin. trial. However, AMD3100 lacks oral bioavailability due to its high overall pos. charge. Initial structure-activity relationship studies with bicyclam analogs suggested that the bis-macrocyclic structure was a prerequisite for anti-HIV activity. Now, we report that the N-pyridinylmethylene cyclam AMD3465, which lacks the structural constraints mentioned above, fully conserves all the biol. properties of AMD3100. Like AMD3100, AMD3465 blocked the cell surface binding of both CXCL12 (the natural CXCR4 ligand), and the specific anti-CXCR4 monoclonal antibody 12G5. AMD3465 dose-dependently inhibited intracellular calcium signaling, chemotaxis, CXCR4 endocytosis and mitogen-activated protein kinase phosphorylation induced by CXCL12. Compared to the bicyclam AMD3100, AMD3465 was even 10-fold more effective as a CXCR4 antagonist, while showing no interaction whatsoever with CCR5. As expected, AMD3465 proved highly potent against X4 HIV strains (IC50: 1-10 nM), but completely failed to inhibit the replication of CCR5-using (R5) viruses. In conclusion, AMD3465 is a novel, monomacrocyclic anti-HIV agent that specifically blocks the

interaction of HIV gp120 with CXCR4. Although oral bioavailability is not yet achieved, the monocyclams, with their decreased mol. charge as compared to the bicyclams, embody an important step forward in the design of oral CXCR4 antagonists that can be clin. used as anti-HIV drugs.

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 4 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:570983 HCAPLUS Full-text
DOCUMENT NUMBER: 143:97274
TITLE: Preparation of piperidines as ***chemokine*** receptor, particularly CCR5, modulators for treatment of inflammatory and autoimmune diseases
INVENTOR(S): ***Bridger, Gary J.***; Zhou, Yuanxi; ***Skerlj, Renato***
PATENT ASSIGNEE(S): Anormed Inc., Can.
SOURCE: PCT Int. Appl., 384 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005059107	A2	20050630	WO 2004-US41865	20041213
WO 2005059107	A3	20060105		
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EP 1708703	A2	20061011	EP 2004-814091	20041213
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PRIORITY APPLN. INFO.: US 2003-528975P P 20031211
WO 2004-US41865 W 20041213

OTHER SOURCE(S): MARPAT 143:97274
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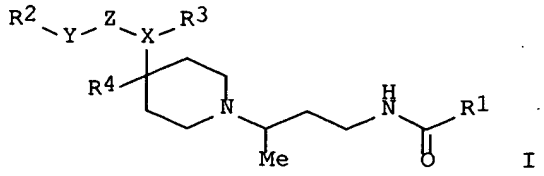

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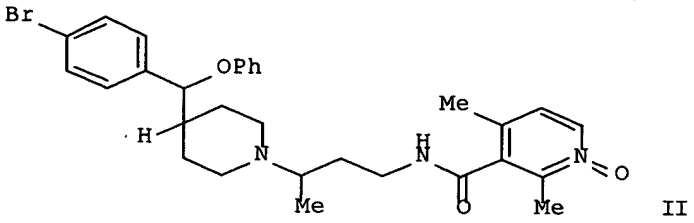

II

AB Title compds. I [wherein X = C, N; Y = O if X = C, or a bond if X = N; Z = (CH2)n; n = 0-1; R1 = (un)substituted hetero/aryl; R2 = (un)substituted hetero/aryl, N:(alkyl); R3 = (un)substituted hetero/aryl, or a Ph fused with a 5- or 6-membered heterocycle; R4 = H, alkyl; and their pharmaceutically acceptable salts] were prepared as ***chemokine*** receptor, particularly CCR5, modulators for treatment of inflammatory and autoimmune diseases. For example, coupling of 2,4-dimethyl-N-oxonicotinic acid with [3-[4-[(4-bromophenyl)phenoxymethyl]piperidin-1-yl]butyl]amine (preparation given) gave II in 82% yield. I exhibited IC50's in the range of 0.01 nM to 50 μM in an assay for inhibition of HIV-1 using PMBC and R5. Compds. I demonstrate protective effects against infection of target cells by a human immunodeficiency virus (HIV).

L32 ANSWER 5 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:1029773 HCAPLUS Full-text
DOCUMENT NUMBER: 142:16292
TITLE: Inhibition of human immunodeficiency virus replication by a dual CCR5/CXCR4 antagonist
AUTHOR(S): Princen, Katrien; Hatse, Sigrid; Vermeire, Kurt; Aquaro, Stefano; De Clercq, Erik; Gerlach, Lars-Ole; Rosenkilde, Mette; Schwartz, Thue W.; ***Skerlj, Renato; Bridger, Gary; Schols, Dominique***
CORPORATE SOURCE: Rega Institute for Medical Research, Louvain, Belg.
SOURCE: Journal of Virology (2004), 78(23), 12996-13006
CODEN: JOVIAM; ISSN: 0022-538X
PUBLISHER: American Society for Microbiology
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Here we report that the N-pyridinylmethylcyclam analog AMD3451 has antiviral activity against a wide variety of R5, R5/X4, and X4 strains of human immunodeficiency virus type 1 (HIV-1) and HIV-2 (50% inhibitory concentration [IC50] ranging from 1.2 to 26.5 μM) in various T-cell lines, CCR5- or CXCR4-transfected cells, peripheral blood mononuclear cells (PBMCs), and monocytes/macrophages. AMD3451 also inhibited R5, R5/X4, and X4 HIV-1 primary clin. isolates in PBMCs (IC50, 1.8 to 7.3 μM). A PCR-based viral entry assay

revealed that AMD3451 blocks R5 and X4 HIV-1 infection at the virus entry stage. AMD3451 dose-dependently inhibited the intracellular Ca2+ signaling induced by the CXCR4 ligand CXCL12 in T-lymphocytic cells and in CXCR4-transfected cells, as well as the Ca2+ flux induced by the CCR5 ligands CCL5, CCL3, and CCL4 in CCR5-transfected cells. The compound did not interfere with ***chemokine***-induced Ca2+ signaling through CCR1, CCR2, CCR3, CCR4, CCR6, CCR9, or CXCR3 and did not induce intracellular Ca2+ signaling by itself at concns. up to 400 μM. In freshly isolated monocytes, AMD3451 inhibited the Ca2+ flux induced by CXCL12 and CCL4 but not that induced by CCL2, CCL3, CCL5, and CCL7. The CXCL12- and CCL3-induced chemotaxis was also dose-dependently inhibited by AMD3451. Furthermore, AMD3451 inhibited CXCL12- and CCL3L1-induced endocytosis in CXCR4- and CCR5-transfected cells. AMD3451, in contrast to the specific CXCR4 antagonist AMD3100, did not inhibit but enhanced the binding of several anti-CXCR4 monoclonal antibodies (such as clone 12G5) at the cell surface, pointing to a different interaction with CXCR4. AMD3451 is the first low-mol.-weight anti-HIV agent with selective HIV coreceptor, CCR5 and CXCR4, interaction.

REFERENCE COUNT: 65 THERE ARE 65 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 6 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:927021 HCAPLUS Full-text
DOCUMENT NUMBER: 141:395421
TITLE: Preparation of cis-2,6-di(pyridyl)piperidines and other cis-di(heteroaryl)-substituted azaheterocycles as binding agents for CXCR4 and other ***chemokine*** receptors for treatment of HIV, rheumatoid arthritis, and other diseases and for stimulating progenitor and stem cells
INVENTOR(S): ***Bridger, Gary J.; McEachern, Ernest J.; Skerlj, Renato; Schols, Dominique***
PATENT ASSIGNEE(S): Anormed Inc., Can.
SOURCE: PCT Int. Appl., 221 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004093817	A2	20041104	WO 2004-US12627	20040422
WO 2004093817	A3	20050428		
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AU 2004232361	A1	20041104	AU 2004-232361	20040422
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EP 1615633	A2	20060118	EP 2004-760161	20040422

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CN 1777423	A	20060524	CN 2004-80010845		20040422	
NO 2005004405	A	20060119	NO 2005-4405		20050922	
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			US 2003-505230P	P	20030922	
			WO 2004-US12627	A	20040422	

OTHER SOURCE(S): MARPAT 141:395421

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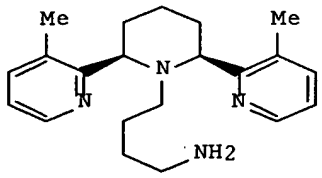


II

AB Cis-di(heteroaryl)-substituted azaheterocycle compds. A-C(B)-L-Y I [A, B = (un)substituted five- or six-membered heteroaryl moiety containing a nitrogen atom next to the bond to ring C; C = (un)substituted partially or fully saturated azaheterocycle with 5-8 ring atoms; L = (un)substituted alkanediyl, alkenediyl, alkynediyl; Y = H, (un)substituted alkyl which may contain heteroatoms, (un)substituted cyclic group; at least one of A or B must be substituted when C is either a piperidinyl or 1,2,3,6-tetrahydropyridinyl ring, and both A and B may not be substituted with naphthalenyl groups if A and B are pyridinyl groups and if C is a piperidinyl moiety; if L-Y is Me, C is not 4-oxo-3,5-piperidinedicarboxylic acid, and if L-Y is benzyl, C is not a 4-hydroxy-1,2,5,6-tetrahydro-3-pyridinecarboxylic acid ester] such as II are prepared as agents capable of binding to ***chemokine*** receptors (particularly the CXCR4 receptor) for treatment of a variety of conditions such as HIV infection, cancer, inflammation, rheumatoid arthritis, immune system disorders, or diseases requiring stimulation of progenitor or stem cells for treatment. Lithium-bromine exchange of 2-bromo-3-methylpyridine followed by addition of the pyridyllithium to di-Me glutarate yields 1,5-bis(3-methyl-2-pyridinyl)-1,5-pentanedione; reduction of the dione with sodium borohydride in methanol to the dipyridinylpentanediol, dimesylation, substitution and cyclization with allylamine and separation of the cis- and trans-piperidines, palladium-mediated N-deallylation, alkylation of the piperidine nitrogen with 4-(N-phthalimidyl)-1-bromobutane, and hydrazine-mediated cleavage of the phthalimide yields II. Compds. I inhibit HIV replication with IC50 values between 0.5 nM and 5 μM, and inhibit SDF-1α-induced calcium flux with IC50 values between 0.5 nM and 5 μM (no data). Compds. of the invention increase and mobilize mouse and human progenitor cells, increase white blood cell count in HIV-infected people, and mobilize CD34-pos. cells in humans; in addition, compds. of the invention mobilize bone marrow cells to repair heart muscle (no data).

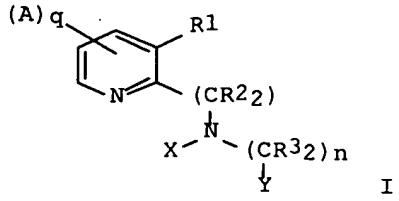
L32 ANSWER 7 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:878165 HCAPLUS Full-text
DOCUMENT NUMBER: 141:379809
TITLE: Preparation of pyridine derivatives as CXCR4 ***chemokine*** receptor binding compounds
INVENTOR(S): ***Bridger, Gary; McEachern, Ernest J. ; Skerlj, Renato; Schols, Dominique***
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 211 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

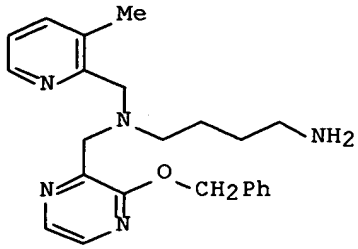
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004209921	A1	20041021	US 2004-823494	20040412
CA 2520259	AA	20041028	CA 2004-2520259	20040412
WO 2004091518	A2	20041028	WO 2004-US11328	20040412
WO 2004091518	A3	20041223		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1613613	A2	20060111	EP 2004-759481	20040412
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				

PRIORITY APPLN. INFO.: US 2003-462736P P 20030411
US 2003-505688P P 20030923
WO 2004-US11328 W 20040412

OTHER SOURCE(S): MARPAT 141:379809
GI



I



II

AB Title compds. I [X = (CR32)o-(CR3=CR3)p-(CR32)r-NR52, (CR32)s-R4, (un)substituted mono or bicyclic ring optionally containing N, O or S, etc.; Y = (un)substituted N-containing monocyclic or bicyclic aromatic or partially aromatic moiety; A and R1 = non-interfering substituent provided that two As do not form a ring; R2 and R3 = H or (un)substituted alkyl; R4 = (un)substituted heterocycle or a hetero compound; R5 = H or alkyl; wherein R1 and R2 is not H; and wherein R1 and R2 may be connected to form an addnl. ring if Y does not contain a 2-imidazoyl residue optionally connected to an addnl. ring; q and n independently = 0-4; p = 0-1; o and r independently = 1-4; s = 1-6 provided that if X = (CR3)2-R4, r is at least two if R4 = 2-pyridinyl, quinolinyl, imidazolyl or furan], as well as their pharmaceutically acceptable salts, are prepared and disclosed as having the ability to bind to ***chemokine*** receptors, in particular CXCR4. Thus, e.g., II was prepared by reductive amination of {4-[(3-methylpyridin-2-ylmethyl)-amino]- butyl}carbamic acid tert-Bu ester (preparation given) with 3-benzyloxypyrazine- 2-carbaldehyde. The present invention also relates to methods of using such compds., such as in treating HIV infection and inflammatory conditions such as rheumatoid arthritis. In assays to evaluate inhibition of HIV-1, many compds. of the invention exhibited IC50 values in the range of 0.5nM-5μM. Furthermore, the present invention relates to methods to elevate progenitor and stem cell counts, as well as methods to elevate white blood cell counts, using such compds.

L32 ANSWER 8 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:773617 HCAPLUS Full-text
DOCUMENT NUMBER: 142:147877
TITLE: Safety, Pharmacokinetics, and Antiviral Activity of AMD3100, a Selective CXCR4 Receptor Inhibitor, in HIV-1 Infection
AUTHOR(S): Hendrix, Craig W.; Collier, Ann C.; Lederman, Michael M.; ***Schols, Dominique***; Pollard, Richard B.; Brown, Stephen; Brooks Jackson, J.; Coombs, Robert W.; Glesby, Marshall J.; Flexner, Charles W.; ***Bridger, Gary J.***; Badel, Karin; MacFarland, Ronald T.; Henson, Geoffrey W.; Calandra, Gary
CORPORATE SOURCE: AMD3100 HIV Study Group, Department of Medicine, Johns

Hopkins University School of Medicine, Baltimore, MD, USA
SOURCE: JAIDS, Journal of Acquired Immune Deficiency Syndromes (2004), 37(2), 1253-1262
CODEN: JJASFJ; ISSN: 1525-4135
PUBLISHER: Lippincott Williams & Wilkins
DOCUMENT TYPE: Journal
LANGUAGE: English

AB AMD3100 is a CXCR4 receptor inhibitor with anti-HIV-1 activity in vitro. We tested the safety, pharmacokinetics, and antiviral effect of AMD3100 administered for 10 days by continuous i.v. infusion in an open-label dose escalation study from 2.5 to 160 μg/kg/h. Forty HIV-infected patients with an HIV RNA level >5000 copies/mL on stable antiretroviral (ARV) regimens or off therapy were enrolled. Syncytium-inducing (SI) phenotype in an MT-2 cell assay was required in higher dose cohorts. Most subjects were black (55%), male (98%), and off ARV therapy. HIV phenotype was SI (30%), non-SI (45%), or not tested (25%). One patient (5 μg/kg/h) had serious and possibly drug-related thrombocytopenia. Two patients (40 and 160 μg/kg/h) had unexpected, although not serious, premature ventricular contractions. Most patients in the 80- and 160-μg/kg/h cohorts had paresthesias. Steady-state blood concentration and area under the concentration-time curve were dose proportional across all dose levels; the median terminal elimination half-life was 8.6 h (range: 8.1-11.1 h). Leukocytosis was observed in all patients, with an estimated maximum effect of 3.4 times baseline (95% confidence interval: 2.9-3.9). Only 1 patient, the patient whose virus was confirmed to use purely CXCR4 and who also received the highest dose (160 μg/kg/h), had a significant 0.9-log10 copies/mL HIV RNA drop at day 11. Overall, however, the average change in viral load across all patients was +0.03 log10 HIV RNA. Given these results, AMD3100 is not being further developed for ARV therapy, but development continues for stem cell mobilization.

REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 9 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:390588 HCAPLUS Full-text
DOCUMENT NUMBER: 141:52717
TITLE: X4 HIV-1 induces neuroblastoma cell death by interference with CXCL12/CXCR4 interaction
AUTHOR(S): Hatse, S.; ***Bridger, G.***; De Clercq, E.; ***Schols, D.***
CORPORATE SOURCE: Laboratory of Virology and Chemotherapy, Rega Institute for Medical Research, Katholieke Universiteit Leuven, Louvain, B-3000, Belg.
SOURCE: Cellular and Molecular Biology (Paris, France, Online) (2003), 49, OL443-OL452
CODEN: CMBPBN; ISSN: 1165-158X
URL: http://www.cellmolbiol.com/page6bis.asp?DOI=10.1170/54
PUBLISHER: CMB Association
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: English

AB Human neuroblastoma SK-N-SH cells strongly express CXC-***chemokine*** receptor 4 (CXCR4), the principal coreceptor for X4 HIV-1 strains, and its natural ligand stromal cell-derived factor 1 (SDF-1, recently renamed CXCL12). The authors investigated the impact of CXCR4 blockade by the specific CXCR4 antagonist AMD3100 or by X4 HIV-1 virus particles on the growth and survival of neuroblastoma SK-N-SH cells. SK-N-SH cell proliferation was inhibited by

AMD3100 and anti-CXCL12 neutralizing antibodies, but enhanced by exogenously added CXCL12. Upon prolonged exposure to AMD3100, SK-N-SH cell death occurred through deficit of survival-promoting and growth-stimulatory signals generated by endogenous CXCL12. In analogy with the observations made with the CXCR4 inhibitor AMD3100, the X4 HIV-1 strains IIIB and SF-2, but not the R5 strain BaL, caused a marked cytopathic effect and strongly effected SK-N-SH cell death after at least 10 days of incubation. However, no virus production could be detected in the HIV-1-inoculated SK-N-SH cell cultures. Exogenously added CXCL12 afforded partial protection against X4 HIV-1-induced cytopathicity in SK-N-SH cells. The data indicate that the endogenous CXCL12/CXCR4 signaling axis is critical for neuroblastoma cell survival and proliferation. Long-term blockade of CXCR4 through phys. contact with the X4 HIV-1 envelope can cause neuronal cell death. This mechanism may possibly play a role in X4 HIV-associated neurodegeneration.

REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 10 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:80349 HCAPLUS Full-text
DOCUMENT NUMBER: 140:146136
TITLE: Preparation of ***chemokine*** receptor binding (benzimidazol-2-ylmethyl)(5,6,7,8-tetrahydroquinolin-8-yl)amines and related heterocyclic compounds with enhanced efficacy against AIDS and other disorders
INVENTOR(S): ***Bridger, Gary***; Kaller, Al; Harwig, Curtis; ***Skerlj, Renato***; Bogucki, David; Wilson, Trevor R.; Crawford, Jason; ***McEachern, Ernest J.***; Atsma, Bem; Nan, Siqiao; Zhou, Yuanxi; ***Schols, Dominique***; Smith, Christopher D.; Di Fluri, Maria R.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 154 pp., Cont.-in-part of U.S. Ser. No. 446,170.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004019058	A1	20040129	US 2003-457034	20030606
US 2003220341	A1	20031127	US 2002-329329	20021223
CA 2522535	AA	20041209	CA 2004-2522535	20040521
WO 2004106493	A2	20041209	WO 2004-US15977	20040521
WO 2004106493	A3	20050825		
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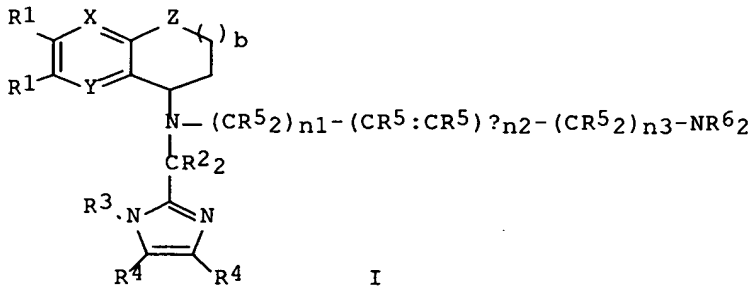
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1628533	A2	20060301	EP 2004-752905	20040521

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR

ZA 2004004589	A	20050909	ZA 2004-4589		20040609
US 2006100240	A1	20060511	US 2005-301725		20051213
PRIORITY APPLN. INFO.:			US 2001-342716P	P	20011221
			US 2002-350822P	P	20020117
			US 2002-329329	A2	20021223
			US 2003-446170	A2	20030523
			US 2003-457034	A	20030606
			WO 2004-US15977	W	20040521

OTHER SOURCE(S): MARPAT 140:146136

GI



I

AB The invention relates to heterocyclic compds. (shown as I; e.g. (1H-benzimidazol-2-ylmethyl)(piperidin-3-ylmethyl)(5,6,7,8- tetrahydroquinolin-8-yl)amine trihydrobromide) consisting of a core N atom surrounded by three pendant groups, wherein two of the three pendant groups are preferably benzimidazolylmethyl and tetrahydroquinolyl, and the 3rd pendant group contains N and optionally contains addnl. rings. The compds. bind to ***chemokine*** receptors, including CXCR4 and CCR5, and demonstrate protective effects against infection of target cells by a human immunodeficiency virus (HIV). Many I exhibit IC50 values of 5-5.5 nM for inhibition of HIV-1 (NL4.3) replication in peripheral blood mononuclear cells and 5 nM-5 μM for inhibition of SDF-1α induced Ca flux in CCRF-CEM cells, a T-lymphoblastoid cell line that expresses CXCR4. It is also stated that the compds. I behave in a manner similar to 1,1'-[1,4-phenylene-bis(methylene)]-bis-1,4,8,11-tetraazacyclotetradecane (AMD3100) which showed to elevate progenitor cell levels (data given). Although the methods of preparation are not claimed, >170 example prepns. are included. For I: X and Y = N or CR1; Z is S, O, NR1 or CR12; each R1-R6 = H or a noninterfering substituent; n1 is 0-4; n2 is 0-1, wherein the a signifies C.tplbond.C may be substituted for CR5:CR5; n3 is 0-4; wherein n1 + n2 + n3 = ≥ 2; b is 0-2; wherein the following combinations of R groups may be coupled to generate a ring, which ring may be (un)saturated: R2 + R2, one R2 + R3, R3 + one R4, R4 + R4, one R5 + another R5, one R5 + one R6, and R6 + R6; wherein the ring may not be aromatic when the participants in ring formation are two R5; and wherein when n2 is 1, neither n1 nor n3 can be 0.

L32 ANSWER 11 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:47834 HCAPLUS Full-text
DOCUMENT NUMBER: 140:144387
TITLE: Molecular Mechanism of AMD3100 Antagonism in the CXCR4 Receptor. Transfer of Binding Site to the CXCR3 Receptor
AUTHOR(S): Rosenkilde, Mette M.; Gerlach, Lars-Ole; Jakobsen, Janus S.; ***Skerlj, Renato T.***; ***Bridger, Gary J.***; Schwartz, Thue W.
CORPORATE SOURCE: Department of Pharmacology, Laboratory for Molecular Pharmacology, University of Copenhagen, The Panum Institute, Copenhagen, DK-2200, Den.
SOURCE: Journal of Biological Chemistry (2004), 279(4), 3033-3041
CODEN: JBCHA3; ISSN: 0021-9258
PUBLISHER: American Society for Biochemistry and Molecular Biology
DOCUMENT TYPE: Journal
LANGUAGE: English
AB AMD3100 is a sym. bicyclam, prototype non-peptide antagonist of the CXCR4 ***chemokine*** receptor. Mutational substitutions at 16 positions located in TM-III, -IV, -V, -VI, and -VII lining the main ligand-binding pocket of the CXCR4 receptor identified three acid residues: Asp171 (AspIV:20), Asp262 (AspVI:23), and Glu288 (GluVII:06) as the main interaction points for AMD3100. Mol. modeling suggests that one cyclam ring of AMD3100 interacts with Asp171 in TM-IV, whereas the other ring is sandwiched between the carboxylic acid groups of Asp262 and Glu288 from TM-VI and -VII, resp. Metal ion binding in the cyclam rings of AMD3100 increased its dependence on Asp262 and provided a tighter mol. map of the binding site, where borderline mutational hits became clear hits for the Zn(II)-loaded analog. The proposed binding site for AMD3100 was confirmed by a gradual build-up in the rather distinct CXCR3 receptor, for which the compound normally had no effect. Introduction of only a Glu at position VII:06 and the removal of a neutralizing Lys residue at position VII:02 resulted in a 1000-fold increase in affinity of AMD3100 to within 10-fold of its affinity in CXCR4. The authors conclude that AMD3100 binds through interactions with essentially only three acidic anchor-point residues, two of which are located at one end and the third at the opposite end of the main ligand-binding pocket of the CXCR4 receptor. The authors suggest that non-peptide antagonists with, for example, improved oral bioavailability can be designed to mimic this interaction and thereby efficiently and selectively block the CXCR4 receptor.
REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 12 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:1012105 HCAPLUS Full-text
DOCUMENT NUMBER: 141:116474
TITLE: The Antiviral Activity of the CXCR4 Antagonist AMD3100 Is Independent of the Cytokine-Induced CXCR4/HIV Coreceptor Expression Level
AUTHOR(S): Princen, Katrien; Hatse, Sigrid; Vermeire, Kurt; ***Bridger, Gary J.***; ***Skerlj, Renato T.***; De Clercq, Erik; ***Schols, Dominique***
CORPORATE SOURCE: Rega Institute for Medical Research, Katholieke Universiteit Leuven, Louvain, B-3000, Belg.
SOURCE: AIDS Research and Human Retroviruses (2003), 19(12), 1135-1139
CODEN: ARHRE7; ISSN: 0889-2229

PUBLISHER: Mary Ann Liebert, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The ***chemokine*** receptor CXCR4 is the main coreceptor used by T-tropic X4 HIV-1 strains to infect its target T cells. It has been proven that the CXCR4 expression level in T cells is strongly up-regulated by interleukin (IL)-4, a Th2-type cytokine that is secreted preferentially in HIV-infected patients in a later stage of disease. This results in an enhancement of HIV-1 replication in CD4+ T-lymphocytes. We have now evaluated the potency of the CXCR4 antagonist AMD3100 in phytohemagglutinin (PHA)/IL-2- vs. PHA/IL-4-activated T cells in order to determine whether the compound has comparable CXCR4-antagonistic and anti-HIV-1 effects under these different cytokine treatments. We analyzed the CXCR4 expression level and the dose-dependent inhibition of CXCR4 expression by AMD3100, by monitoring the binding of an anti-CXCR4 monoclonal antibody (clone 12G5). We also determined stromal cell-derived factor (SDF)-1-induced intracellular calcium signaling and HIV-1 replication in these cells in the absence and presence of AMD3100. The CXCR4 expression level in PHA/IL-4-stimulated cells was much higher than in PHA/IL-2-stimulated cells. However, the potency of the bicyclam AMD3100 to block anti-CXCR4 mAb binding, SDF-1-induced intracellular calcium signaling, and HIV-1 replication of the X4 NL4.3 strain and three primary isolates remained unchanged. Our data indicate that CXCR4 antagonists such as AMD3100 act independently of the HIV-1 coreceptor expression level. These compds. should therefore be useful in suppressing HIV-1 infection in all stages of the disease.

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 13 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:732923 HCAPLUS Full-text
DOCUMENT NUMBER: 139:395792
TITLE: Convenient synthesis of 5,6,7,8-tetrahydroquinolin-8-ylamine and 6,7-dihydro-5H-quinolin-8-one
AUTHOR(S): ***McEachern, E. J.***; Yang, W.; Chen, G.; ***Skerlj, R. T.***; ***Bridger, G. J.***
CORPORATE SOURCE: AnorMED Inc., Langley, BC, Can.
SOURCE: Synthetic Communications (2003), 33(20), 3497-3502
CODEN: SYNCAV; ISSN: 0039-7911
PUBLISHER: Marcel Dekker, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:395792

AB A novel two-step synthesis of 5,6,7,8-tetrahydroquinolin-8-ylamine, involving regioselective nitrosation of 5,6,7,8-tetrahydroquinoline followed by oxime reduction, is described. Oxime hydrolysis affords 6,7-dihydro-5H-quinolin-8-one.

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 14 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:532661 HCAPLUS Full-text
DOCUMENT NUMBER: 139:101128
TITLE: Preparation of ***chemokine*** receptor binding (benzimidazol-2-ylmethyl)(5,6,7,8-tetrahydroquinolin-8-yl)amines and related heterocyclic compounds with enhanced efficacy against AIDS and other disorders
INVENTOR(S): ***Bridger, Gary J.***; ***Skerlj, Renato T.***; Kaller, Al; Harwig, Curtis; Bogucki, David; Wilson, Trevor; Crawford, Jason; ***McEachern, Ernest J.***

; Atsma, Bem; Nan, Siqiao; Zhou, Yuanxi; ***Schols, Dominique***; Smith, Christopher Dennis; Di Fluri, Rosaria Maria

PATENT ASSIGNEE(S): Anormed Inc., Can.; et al.; et al.

SOURCE: PCT Int. Appl., 360 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2003055876	A1	20030710	WO 2002-US41407		20021223
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
CA 2467718	AA	20030710	CA 2002-2467718		20021223
AU 2002357379	A1	20030715	AU 2002-357379		20021223
BR 2002015050	A	20041013	BR 2002-15050		20021223
EP 1465889	A1	20041013	EP 2002-805977		20021223
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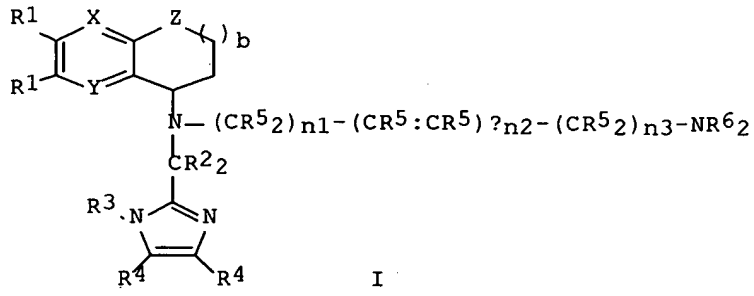
CN 1596255	A	20050316	CN 2002-825638		20021223
JP 2005518397	T2	20050623	JP 2003-556406		20021223
ZA 2004004589	A	20050909	ZA 2004-4589		20040609
NO 2004002578	A	20040907	NO 2004-2578		20040618
PRIORITY APPLN. INFO.:			US 2001-342716P	P	20011221
			US 2002-350822P	P	20020117
			WO 2002-US41407	W	20021223

OTHER SOURCE(S): MARPAT 139:101128

GI



I

AB The invention relates to heterocyclic compds. (shown as I; e.g. (1H-benzimidazol-2-ylmethyl)(piperidin-3-ylmethyl)(5,6,7,8- tetrahydroquinolin-8-yl)amine trihydrobromide) consisting of a core N atom surrounded by three pendant groups, wherein two of the three pendant groups are preferably benzimidazolylmethyl and tetrahydroquinolyl, and the 3rd pendant group contains N and optionally contains addnl. rings. The compds. bind to ***chemokine*** receptors, including CXCR4 and CCR5, and demonstrate protective effects against infection of target cells by a human immunodeficiency virus (HIV). Many I exhibit IC50 values of 5-5.5 nM for inhibition of HIV-1 (NL4.3) replication in peripheral blood mononuclear cells and 5 nM-5 μM for inhibition of SDF-1α induced Ca flux in CCRF-CEM cells, a T-lymphoblastoid cell line that expresses CXCR4. Although the methods of preparation are not claimed, >170 example prepns. are included. For I: X and Y = N or CR1; Z is S, O, NR1 or CR12; each R1-R6 = H or a noninterfering substituent; n1 is 0-4; n2 is 0-1, wherein the a signifies C.tplbond.C may be substituted for CR5:CR5; n3 is 0-4; wherein n1 + n2 + n3 = ≥ 2; b is 0-2; wherein the following combinations of R groups may be coupled to generate a ring, which ring may be (un)saturated: R2 + R2, one R2 + R3, R3 + one R4, R4 + R4, one R5 + another R5, one R5 + one R6, and R6 + R6; wherein the ring may not be aromatic when the participants in ring formation are two R5; and wherein when n2 is 1, neither n1 nor n3 can be 0.

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 15 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:486052 HCAPLUS Full-text
DOCUMENT NUMBER: 139:116135
TITLE: Mutations at the CXCR4 interaction sites for AMD3100 influence anti-CXCR4 antibody binding and HIV-1 entry
AUTHOR(S): Hatse, Sigrid; Princen, Katrien; Vermeire, Kurt; Gerlach, Lars-Ole; Rosenkilde, Mette M.; Schwartz, Thue W.; ***Bridger, Gary***; De Clercq, Erik; ***Schols, Dominique***
CORPORATE SOURCE: Rega Institute for Medical Research, Laboratory of Virology and Chemotherapy, Katholieke Universiteit Leuven, Louvain, B-3000, Belg.
SOURCE: FEBS Letters (2003), 546(2-3), 300-306
CODEN: FEBLAL; ISSN: 0014-5793
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The interaction of the CXCR4 antagonist AMD3100 with its target is greatly influenced by specific aspartate residues in the receptor protein, including Asp171 and Asp262. The authors have now found that aspartate-to-asparagine substitutions at these positions differentially affect the binding of four different anti-CXCR4 monoclonal antibodies as well as the infectivity of diverse human immunodeficiency virus type 1 (HIV-1) strains and clin. isolates. Mutation of Asp262 strongly decreased the coreceptor efficiency of CXCR4 for wild-type but not for AMD3100-resistant HIV-1 NL4.3. Thus, resistance of HIV-1 NL4.3 to AMD3100 is associated with a decreased dependence of the viral gp120 on Asp262 of CXCR4, pointing to a different mode of interaction of wild-type vs. AMD3100-resistant virus with CXCR4.

REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 16 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:242771 HCAPLUS Full-text

DOCUMENT NUMBER: 138:401628
TITLE: Enzymatic Resolution of Bicyclic 1-Heteroarylamines Using Candida antarctica Lipase B
AUTHOR(S): Skupinska, Krystyna A.; ***McEachern, Ernest J.***; Baird, Ian R.; ***Skerlj, Renato T.***; ***Bridger, Gary J.***
CORPORATE SOURCE: AnorMED Inc., Langley, BC, V2Y 1N5, Can.
SOURCE: Journal of Organic Chemistry (2003), 68(9), 3546-3551
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:401628

AB Candida antarctica lipase B has been used to kinetically resolve a structurally diverse series of bicyclic 1-heteroaryl primary amines, e.g. 8-amino-5,6,7,8-tetrahydroquinoline, 5-amino-5,6,7,8- tetrahydroquinoxaline, etc., by enantioselective acetylation. High yields of either enantiomer could be obtained with excellent enantioselectivity (90-99% ee), while the undesired enantiomer could, in some cases, be recycled by thermal racemization. The absolute stereochem. of the products was confirmed by an X-ray crystallog.

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 17 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:221637 HCAPLUS Full-text
DOCUMENT NUMBER: 138:255107
TITLE: Synthesis of enantiomerically pure amino-substituted fused bicyclic rings
INVENTOR(S): ***McEachern, Ernest J.***; ***Bridger, Gary J.***; Skupinska, Krystyna A.; ***Skerlj, Renato T.***
PATENT ASSIGNEE(S): Anormed Inc., Can.
SOURCE: PCT Int. Appl., 85 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

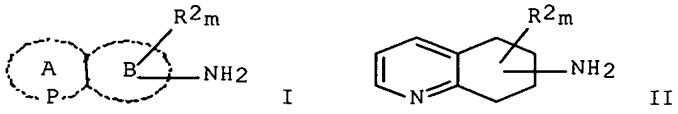
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003022785	A2	20030320	WO 2002-US29372	20020912
WO 2003022785	A3	20040930		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2456614	AA	20030320	CA 2002-2456614	20020912
US 2003114679	A1	20030619	US 2002-243434	20020912
US 6825351	B2	20041130		
EP 1487795	A2	20041222	EP 2002-775823	20020912
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				

IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK

BR 2002012443	A	20050315	BR 2002-12443	20020912
JP 2005508316	T2	20050331	JP 2003-526864	20020912
CN 1608052	A	20050420	CN 2002-817593	20020912
CN 1817864	A	20060816	CN 2006-10005453	20020912
ZA 2004000750	A	20050406	ZA 2004-750	20040129
NO 2004001012	A	20040310	NO 2004-1012	20040310
US 2005080267	A1	20050414	US 2004-959823	20041006
PRIORITY APPLN. INFO.:			US 2001-323201P	P 20010912
			CN 2002-817593	A3 20020912
			US 2002-243434	A3 20020912
			WO 2002-US29372	W 20020912

OTHER SOURCE(S): MARPAT 138:255107

GI



AB This invention describes various processes for synthesis and resolution of racemic amino-substituted fused bicyclic ring systems (shown as I; variables defined below), primarily 5,6,7,8-tetrahydroquinolines (shown as II; e.g. 8-amino-2-methyl-5,6,7,8-tetrahydroquinoline) and 5,6,7,8-tetrahydroisoquinolines (e.g. 5-amino-5,6,7,8- tetrahydroisoquinoline). One process uses selective hydrogenation of an amino-substituted fused bicyclic aromatic ring system; for example, 8-amino-5,6,7,8-tetrahydroquinoline was obtained in 2 steps (100, 54 and 91% yields) from 8-aminoquinoline via intermediates 8-acetylaminoquinoline and 8-acetylamino-5,6,7,8-tetrahydroquinoline using PtO2/trifluoroacetic acid/H2 for the hydrogenation. An alternative process preps. the racemic amino-substituted fused bicyclic ring system via nitrosation; for example, 5,6,7,8-tetrahydroquinoline was converted with LDA/MTBE at -30° followed by isoamyl nitrite to 8-hydroxyimino-5,6,7,8-tetrahydroquinoline (75%) that was hydrogenated using H2/Pd/C/MeOH to give 8-amino-5,6,7,8-tetrahydroquinoline (100%). The present invention describes the enzymic resolution of a racemic mixture to produce the (R)- and (S)- forms of amino-substituted fused bicyclic rings as well as a racemization process to recycle the unpreferred enantiomer. For example, 8-amino-5,6,7,8-tetrahydroquinoline was half reacted with EtOAc in iPr2O at 60° in the presence of Candida antarctica lipase to give (R)-(-)-N-(5,6,7,8-tetrahydroquinolin-8-yl)acetamide (97% ee) and unreacted (S)-(+)-8-amino-5,6,7,8-tetrahydroquinoline (96% ee). The amine could be racemized at 150° in a sealed tube under Ar with 87% yield. Further provided by this invention is an asym. synthesis of the (R)- or (S)- enantiomer of primary amino-substituted fused bicyclic ring systems. For example, (R)-(-)-8-amino-5,6,7,8-tetrahydroquinoline (98% ee) was obtained in 4 steps (82, 95, 93 and 59% yields) starting from 8-hydroxy-5,6,7,8-tetrahydroquinoline via intermediates 6,7-dihydro-5H-quinolin-8-one, (R)-(-)-(6,7-dihydro-5H-quinolin-8- ylidene)(1-phenylethyl)amine, and (-)-((1R)-1-Phenylethyl)-(8-(R)-5,6,7,8-tetrahydroquinolin-8-yl)amine using (R)-(+)-α-methylbenzylamine as chiral auxiliary. For I: ring A is a heteroarom. 5- or 6-membered ring, P is N, S or O; ring B is a 5- or 6-membered cycloalkyl or heterocycloalkyl; NH2 is located

at a position on ring B; and R2 is located at any other H position on the fused bicyclic ring; m is 0-4; R2 = halo, nitro, cyano, carboxylic acid, alkyl, alkenyl, cycloalkyl, hydroxy, thiol, a protected amino, acyl, carboxylate, carboxamide, sulfonamide, an aromatic group and a heterocyclic group. The variable definitions for II and the isoquinolines are the same as for I.

L32 ANSWER 18 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:35359 HCAPLUS Full-text
DOCUMENT NUMBER: 138:106725
TITLE: Preparation of antiviral macrocyclic polyamines
INVENTOR(S): ***Bridger, Gary James***; Boehringer, Eva Maria; Wang, Zhongren; ***Schols, Dominique***; ***Skerlj, Renato Tony***; Bogucki, David Earl
PATENT ASSIGNEE(S): Anormed, Inc., Can.
SOURCE: U.S., 18 pp., Cont.-in-part of U.S. 5,817,807.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6506770	B1	20030114	US 1998-111895	19980708
US 5817807	A	19981006	US 1996-659500	19960606
CA 2336634	AA	20000120	CA 1999-2336634	19990708
WO 2000002870	A1	20000120	WO 1999-CA619	19990708
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9945959	A1	20000201	AU 1999-45959	19990708
AU 767359	B2	20031106		
BR 9912524	A	20010502	BR 1999-12524	19990708
EP 1095031	A1	20010502	EP 1999-928956	19990708
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
TR 200100030	T2	20010621	TR 2001-200100030	19990708
JP 2002520323	T2	20020709	JP 2000-559101	19990708
NZ 509699	A	20031031	NZ 1999-509699	19990708
CN 1679562	A	20051012	CN 2005-10009486	19990708
NO 2001000047	A	20010301	NO 2001-47	20010104
US 6872714	B1	20050329	US 2001-743561	20010813
US 2003018189	A1	20030123	US 2002-143692	20020509
US 6756391	B2	20040629		
US 2004235814	A1	20041125	US 2004-872735	20040621
US 2005154005	A1	20050714	US 2004-991944	20041117
PRIORITY APPLN. INFO.:			US 1996-659500	A2 19960606
			GB 1995-11357	A 19950606
			US 1998-111895	A 19980708
			CN 1999-808260	A3 19990708
			WO 1999-CA619	W 19990708

US 2001-743561 A1 20010813
US 2002-143692 A1 20020509

OTHER SOURCE(S): MARPAT 138:106725

AB Monocyclic polyamines V-CR1R2-Ar-CR3R4-NR5-(CR6R7)x-R8 [wherein V = cyclic polyamine having a total of 9-24 members; R1-R7 = independently H, (cyclo)alkyl; R8 = heterocyclic group, aromatic group, SH; Ar = (un)substituted (hetero)aromatic ring; x = 1, 2], which showed activity in standard tests against HIV-infected cells as well as other biol. activity related to binding of ligands to ***chemokine*** receptors, were prepared For example, 4,8,11-tris(diethoxyphosphoryl)-1,4,8,11- tetraazacyclotetradecane was coupled with α,α'-dibromo-p- xylene, alkylated, and deprotected using HBr/HOAc to give N-[1,4,8,11-tetraazacyclotetradecanyl-1,4-phenylenebis(methylene)]-2- (aminomethyl)pyridine•6HBr (AMD3465). The latter strongly inhibited HIV-1 with an EC50 value of 0.008 μg/mL and displayed low cytotoxicity toward MT-4 HIV challenged cells with a CC50 value of > 250 μ/mL. In addition, a selectivity index, corresponding to the ratio of CC50 to EC50, of 3x104 for AMD3465 indicates high potential for therapeutic use.

REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 19 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:42 HCAPLUS Full-text
DOCUMENT NUMBER: 138:165456
TITLE: Metal Ion Enhanced Binding of AMD3100 to Asp262 in the CXCR4 Receptor
AUTHOR(S): Gerlach, Lars Ole; Jakobsen, Janus S.; Jensen, Kasper P.; Rosenkilde, Mette R.; ***Skerlj, Renato T.***; Ryde, Ulf; ***Bridger, Gary J.***; Schwartz, Thue W.
CORPORATE SOURCE: Laboratory for Molecular Pharmacology, University of Copenhagen, Copenhagen, Den.
SOURCE: Biochemistry (2003), 42(3), 710-717
CODEN: BICHAW; ISSN: 0006-2960
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The affinity of AMD3100, a sym. nonpeptide antagonist composed of two 1,4,8,11-tetraazacyclotetradecane (cyclam) rings connected through a 1,4-dimethylene(phenylene) linker to the CXCR4 ***chemokine*** receptor was increased 7, 36, and 50-fold, resp., by incorporation of the following: Cu2+, Zn2+, or Ni2+ into the cyclam rings of the compound The rank order of the transition metal ions correlated with the calculated binding energy between free acetate and the metal ions coordinated in a cyclam ring. Construction of AMD3100 substituted with only a single Cu2+ or Ni2+ ion demonstrated that the increase in binding affinity of the metal ion substituted bicyclam is achieved through an enhanced interaction of just one of the ring systems. Mutational anal. of potential metal ion binding residues in the main ligand binding crevice of the CXCR4 receptor showed that although binding of the bicyclam is dependent on both Asp171 and Asp262, the enhancing effect of the metal ion was selectively eliminated by substitution of Asp262 located at the extracellular end of TM-VI. It is concluded that the increased binding affinity of the metal ion substituted AMD3100 is obtained through enhanced interaction of one of the cyclam ring systems with the carboxylate group of Asp262. It is suggested that this occurs through a strong concomitant interaction of one of the oxygen's directly with the metal ion and the other oxygen to one of the nitrogens of the cyclam ring through a hydrogen bond.

REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 20 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:746521 HCAPLUS Full-text
DOCUMENT NUMBER: 138:13999
TITLE: Concise Preparation of Amino-5,6,7,8-tetrahydroquinolines and Amino-5,6,7,8-tetrahydroisoquinolines via Catalytic Hydrogenation of Acetamidoquinolines and Acetamidoisoquinolines
AUTHOR(S): Skupinska, Krystyna A.; ***McEachern, Ernest J.***; ***Skerlj, Renato T.***; ***Bridger, Gary J.***
CORPORATE SOURCE: AnorMED Inc., Langley, BC, V2Y 1N5, Can.
SOURCE: Journal of Organic Chemistry (2002), 67(22), 7890-7893
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:13999
AB A method to prepare amino-substituted 5,6,7,8-tetrahydroquinolines and 5,6,7,8-tetrahydroisoquinolines via catalytic hydrogenation of the corresponding acetamido-substituted quinolines and isoquinolines followed by acetamide hydrolysis is described. The yields of the products are good when the acetamido substituent is present on the pyridine ring and moderate with the acetamido substituent on the benzene ring. This method has also been applied to the regioselective reduction of quinoline substrates bearing other substituents (R = OMe, CO2Me, Ph).
REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 21 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:684699 HCAPLUS Full-text
DOCUMENT NUMBER: 138:265565
TITLE: ***Chemokine*** receptor inhibition by AMD3100 is strictly confined to CXCR4
AUTHOR(S): Hatse, Sigrid; Princen, Katrien; ***Bridger, Gary***; De Clercq, Erik; ***Schols, Dominique***
CORPORATE SOURCE: Rega Institute for Medical Research, Laboratory of Virology and Chemotherapy, Katholieke Universiteit Leuven, Louvain, B-3000, Belg.
SOURCE: FEBS Letters (2002), 527(1-3), 255-262
CODEN: FEBLAL; ISSN: 0014-5793
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB This study was undertaken to demonstrate the unique specificity of the ***chemokine*** receptor CXCR4 antagonist AMD3100. Calcium flux assays with selected ***chemokine***/cell combinations, affording distinct ***chemokine*** receptor specificities, revealed no interaction of AMD3100 with any of the ***chemokine*** receptors CXCR1 through CXCR3, or CCR1 through CCR9. In contrast, AMD3100 potently inhibited CXCR4-mediated calcium signaling and chemotaxis in a concentration-dependent manner in different cell types. Also, AMD3100 inhibited stromal cell-derived factor (SDF)-1-induced endocytosis of CXCR4, but did not affect phorbol ester-induced receptor internalization. Importantly, AMD3100 by itself was unable to elicit intracellular calcium fluxes, to induce chemotaxis, or to trigger CXCR4 internalization, indicating that the compound does not act as a CXCR4 agonist. Specific small-mol. CXCR4 antagonists such as AMD3100 may play an important role in the treatment of

human immunodeficiency virus infections and many other pathol. processes that are dependent on SDF-1/CXCR4 interactions (e.g. rheumatoid arthritis, atherosclerosis, asthma and breast cancer metastasis).

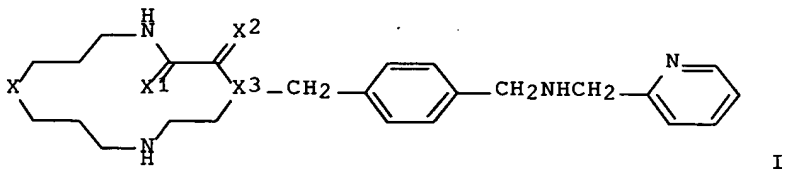
REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 22 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:466711 HCAPLUS Full-text
DOCUMENT NUMBER: 137:47236
TITLE: Preparation of pyridylmethylaminomethylbenzyltriazacyclotetradecanes as ***chemokine*** receptor antagonists
INVENTOR(S): ***Bridger, Gary***; Boehringer, Eva Maria; Wang, Zhongren; ***Schols, Dominique***; ***Skerlj, Renato T.***; Bogucki, David E.
PATENT ASSIGNEE(S): Anormed, USA
SOURCE: U.S. Pat. Appl. Publ., 23 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002077339	A1	20020620	US 2000-740050	20001215
US 6667320	B2	20031223		
US 2004102428	A1	20040527	US 2003-703781	20031107
US 7022717	B2	20060404		
US 2006069129	A1	20060330	US 2005-281296	20051116

PRIORITY APPLN. INFO.:
US 1999-172153P P 19991217
US 2000-740050 A1 20001215
US 2003-703781 A1 20031107

OTHER SOURCE(S): MARPAT 137:47236
GI



I

AB Monocyclic polyamines I [X = CHF, CF2, O, S, SO, SO2, X1, X2 = H2, X3 = N; X = CH2, X1 = O, X2 = H2, X3 = N; X = CH2, X1 = H2, X2 = O, X3 = N; X = O, X1, X2 = H2, X = CH] were prepared and have activity in standard tests against HIV- or FIV- infected cells as well as other biol. activity related to binding of ligands to ***chemokine*** receptors that mediate a number of mammalian embryonic developmental processes. Thus, I [X = N, X1, X2 = H2, X3 = N] was prepared from FCH[(CH2)3OTs]2 and (2- O2NC6H4SO2NHCH2CH2)2NP(O)(OEt)2 to form the macrocycle which was deblocked and treated with the N-protected bromide of the side chain, followed by deblocking.

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

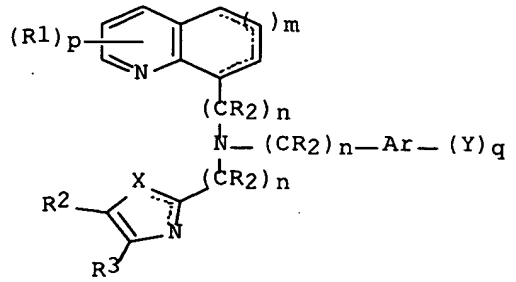
L32 ANSWER 23 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:355048 HCAPLUS Full-text
DOCUMENT NUMBER: 137:362819
TITLE: AMD3100, a CxCR4 antagonist, attenuates allergic lung inflammation and airway hyperreactivity
AUTHOR(S): Lukacs, Nicholas W.; Berlin, Aaron; ***Schols, Dominique***; ***Skerlj, Renato T.***; ***Bridger, Gary J.***
CORPORATE SOURCE: Department of Pathology, University of Michigan Medical School, Ann Arbor, MI, 48109-0602, USA
SOURCE: American Journal of Pathology (2002), 160(4), 1353-1360
CODEN: AJPAA4; ISSN: 0002-9440
PUBLISHER: American Society for Investigative Pathology
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The role of specific ***chemokine*** receptors during allergic asthmatic responses has been relatively undefined. A number of receptors are preferentially expressed on Th2 cells, including CCR4, CCR8, and CxCR4. In the present study, we have examined the role of CxCR4 in the development of cockroach allergen-induced inflammation and airway hyperreactivity in a mouse model of asthma. Using a specific inhibitor of CxCR4, AMD3100, our results indicate that blocking this receptor has a significant effect in down-regulating the inflammation and pathophysiol. of the allergen-induced response. Treatment of allergic mice with AMD3100 significantly reduced airway hyperreactivity, peribronchial eosinophilia, and the overall inflammatory responses. In addition, there was a shift in the cytokine profile that was observed in the AMD3100-treated animals. Specifically, there was a significant reduction in interleukin-4 and interleukin-5 levels and a significant increase in interleukin-12 and interferon-γ levels within the lungs of treated allergic mice. Furthermore, there was a significant alteration in the local ***chemokine*** production of CCL22 (MDC) and CCL17 (TARC), two ***chemokines*** previously shown to be important in Th2-type allergen responses. Overall, specifically blocking CxCR4 using AMD3100 reduced a number of pathol. parameters related to asthmatic-type inflammation.
REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 24 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:332188 HCAPLUS Full-text
DOCUMENT NUMBER: 136:355235
TITLE: Preparation of tertiary N-(5,6,7,8-tetrahydro-8-quinolinyl)-N-(1H-benzimidazol-2-ylmethyl)amines and analogs as ***chemokine*** receptor modulators for treatment of HIV or FIV
INVENTOR(S): ***Bridger, Gary***; ***Skerlj, Renato***; Kaller, Al; Harwig, Curtis; Bogucki, David; Wilson, Trevor R.; Crawford, Jason; ***Mceachern, Ernest J.***; Atsman, Berm; Nan, Siqiao; Zhou, Yuanxi; ***Schols, Dominique***; Smith, Christopher Dennis; Di Fluri, Rosaria Maria
PATENT ASSIGNEE(S): Anormed Inc., Can.
SOURCE: PCT Int. Appl., 187 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent

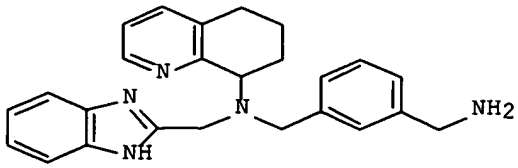
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2002034745	A1	20020502	WO 2001-US29590		20010919
WO 2002034745	C1	20030918			
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
CA 2421796	AA	20020502	CA 2001-2421796		20010917
EP 1317451	A1	20030611	EP 2001-975290		20010917
EP 1317451	B1	20060809			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
BR 2001013932	A	20030624	BR 2001-13932		20010917
NZ 524651	A	20050826	NZ 2001-524651		20010917
AT 335733	E	20060915	AT 2001-975290		20010917
AU 2001094628	A5	20020506	AU 2001-94628		20010919
JP 2004512336	T2	20040422	JP 2002-537736		20010919
US 2003028022	A1	20030206	US 2002-31812		20020328
US 6734191	B2	20040511			
NO 2003001161	A	20030313	NO 2003-1161		20030313
US 2004171638	A1	20040902	US 2004-799386		20040311
US 7091217	B2	20060815			
US 2004220207	A1	20041104	US 2004-858910		20040601
US 7084155	B2	20060801			
US 2005026942	A1	20050203	US 2004-914663		20040809
US 2006128750	A1	20060615	US 2006-345987		20060202
PRIORITY APPLN. INFO.:			US 2000-234510P	P	20000922
			US 2000-234816P	P	20000922
			US 2000-232891P	P	20000915
			US 2000-233087P	P	20000915
			US 2001-957654	A3	20010917
			US 2001-957682	A3	20010917
			WO 2001-US29590	W	20010919
			US 2002-31812	A1	20020328
			US 2004-858910	A3	20040601

OTHER SOURCE(S): MARPAT 136:355235
GI



I



II

AB Title compds. I [wherein ring A optionally comprises a heteroatom selected from N, O, or S; R1-R3 = non-interfering substituents; R4 and R5 = independently H or (un)substituted alkyl, alkenyl, alkynyl, or acyl; or 2 R5 may form a cyclic amine, optionally containing 1 or more N, O, and/or S; R = independently H or alkyl; X = O or S or (un)substituted C or N; Y = independently halo, OH, SH, SO, SO2, non-N containing organic moiety, (CH2)xCN, (CR2)xNR52, (CR2)xNR(CR2)xNRR4, (CR2)xNR(CR2)xNR(CR2)xNR52, (CR2)xCO(CR2)xNR52, (CR2)xCO(CR2)xNR(CR2)xNRR4, (CR2)xCO(CR2)xNR(CR2)xNR(CR2)xNR52, (CR2)xNRCO(CR2)xNRR4, (CR2)xNRCO(CR2)xNR(CR2)xNR52, (CR2)xNRCO(CR2)xNR(CR2)xNR(CR2)xNR(CR2)xNR52 , CH:NZ, (CR2)xZ, NR(CR2)xZ, (CR2)xNROH, (CR2)xCONROH, or (CR2)xCR:NOH; or 2 Y groups may be connected to form a fused ring with Ar; Z = (un)substituted (hetero)aryl; Ar = (hetero)aryl; m = 0-2; n = 0-2; p = 0-4; q = 0-3; x = 0-4; with provisos; and pharmaceutically acceptable salts and pro-drugs thereof] were prepared as modulators of ***chemokine*** receptor activities. For example, reductive addition of 3-cyanobenzaldehyde to 8-amino-5,6,7,8-tetrahydroquinoline using sodium triacetoxyborohydride in CH2Cl2 afforded N-(5,6,7,8-tetrahydro-8- quinolinyl)-3-cyanobenzylamine (81%). Alkylation with N-(tert-butoxycarbonyl)-2-chloromethylbenzimidazole using N,N-diisopropylethylamine and KI in MeCN (88%), followed by hydrogenation in the presence of Raney nickel (79%), gave the tertiary amine II (AMD9679). Compds. of the invention tested for inhibition of HIV-1 NL4.3 or IIIB replication in MT-4 cells exhibited EC50 values of 0.002 μM/mL to 20.0 μM/mL. Thus, I are useful for the treatment of human immunodeficiency virus (HIV) and/or feline immunodeficiency virus (FIV).

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 25 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:220576 HCAPLUS Full-text
DOCUMENT NUMBER: 136:263160
TITLE: Preparation of azolylmethylaminotetrahydroquinolines and related compounds as ***chemokine*** receptor binding agents.
INVENTOR(S): ***Bridger, Gary; Skerlj, Renato;*** Kaller, Al; Harwig, Curtis; Bogucki, David; Wilson,

Trevor R.; Crawford, Jason; ***McEachern, Ernest J.***; Atsma, Bem; Nan, Siqiao; Zhou, Yuanxi; ***Schols, Dominique***; Smith, Christopher Dennis; Di, Fluri Rosaria Maria

PATENT ASSIGNEE(S): Anormed Inc., Can.
SOURCE: PCT Int. Appl., 254 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2002022600	A2	20020321	WO 2001-CA1326		20010917
WO 2002022600	A3	20020510			
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
CA 2419224	AA	20020321	CA 2001-2419224		20010917
AU 2001091569	A5	20020326	AU 2001-91569		20010917
US 2003018046	A1	20030123	US 2001-957682		20010917
US 6864265	B2	20050308			
EP 1317445	A2	20030611	EP 2001-971574		20010917
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
BR 2001013930	A	20030624	BR 2001-13930		20010917
TR 200300322	T2	20030922	TR 2003-322		20010917
JP 2004508422	T2	20040318	JP 2002-526853		20010917
NZ 524420	A	20050429	NZ 2001-524420		20010917
AT 335733	E	20060915	AT 2001-975290		20010917
ZA 2003001398	A	20040521	ZA 2003-1398		20030220
ZA 2003001402	A	20050120	ZA 2003-1402		20030220
NO 2003001179	A	20030314	NO 2003-1179		20030314
US 2004171638	A1	20040902	US 2004-799386		20040311
US 7091217	B2	20060815			
US 2004220207	A1	20041104	US 2004-858910		20040601
US 7084155	B2	20060801			
US 2006128750	A1	20060615	US 2006-345987		20060202
PRIORITY APPLN. INFO.:			US 2000-232891P	P	20000915
			US 2000-234510P	P	20000922
			US 2000-233087P	P	20000915
			US 2000-234816P	P	20000922
			US 2001-957682	A3	20010917
			WO 2001-CA1326	W	20010917
			US 2002-31812	A1	20020328
			US 2004-858910	A3	20040601

OTHER SOURCE(S): MARPAT 136:263160
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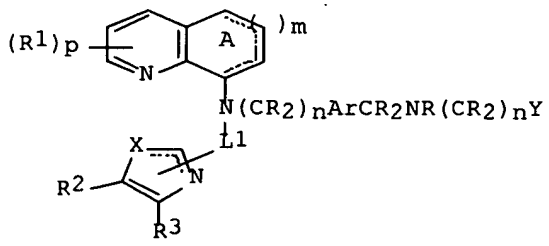

I

AB Title compds. [I; ring A optionally contains N, O, S; dotted lines = optional unsatn.; R1, R2, R3 = non-interfering substituents; p = 0-4; m = 0-2; L1 = linker of 1.5-10 Å; X = O, S, (substituted) C, N; Ar = aryl; n = 0-2; R = H, alkyl; Y = aryl, heteroaryl, heterocyclyl], were prepared Thus, 5-trifluoromethyl-2-chloromethylbenzimidazole (preparation given), N-(tert-butoxycarbonyl)-N-(2-pyridinylmethyl)-N'-(5,6,7,8-tetrahydro-8- quinolinyl)-1,4-benzenedimethanamine, and diisopropylethylamine were stirred at 80° in DMF for 16 h to yield N-(tert-butoxycarbonyl)-N- (2-pyridinylmethyl)-N'-(5-trifluoromethyl-1H-benzimidazol-2-ylmethyl)-N'- (5,6,7,8-tetrahydro-8-quinolinyl)-1,4-benzenedimethanamine. Deprotection with HBr in HOAc or dioxane gave N-(2-pyridinylmethyl)-N'-(5- trifluoromethyl-1H-benzimidazol-2-ylmethyl)-N'-(5,6,7,8-tetrahydro-8- quinolinyl)-1,4-benzenedimethanamine hydrobromide. Several I inhibited HIV-1 replication in MT-4 cells with EC50<20 μg/mL.

L32 ANSWER 26 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:220575 HCAPLUS Full-text
DOCUMENT NUMBER: 136:263159
TITLE: ***Chemokine*** receptor-binding heterocyclic compounds, particularly (5,6,7,8-tetrahydroquinolin-8-yl)amino- and (1H-benzimidazol-2-yl)methyl-containing aromatic and heteroaromatic amides, useful for treating infection with HIV and FIV
INVENTOR(S): ***Bridger, Gary; Skerlj, Renato;*** Kaller, Al; Harwig, Curtis; Bogucki, David; Wilson, Trevor R.; Crawford, Jason; ***McEachern, Ernest J.***; Atsma, Bem; Nan, Siqiao; Zhou, Yuanxi; ***Schols, Dominique***; Smith, Christopher Dennis; Di Fluri, Rosaria Maria
PATENT ASSIGNEE(S): Anormed Inc., Can.
SOURCE: PCT Int. Appl., 146 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002022599	A2	20020321	WO 2001-CA1325	20010917
WO 2002022599	A3	20020530		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,

GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2419219	AA	20020321	CA 2001-2419219	20010917
AU 2001093551	A5	20020326	AU 2001-93551	20010917
US 2002147192	A1	20021010	US 2001-957654	20010917
US 6835731	B2	20041228		
EP 1317443	A2	20030611	EP 2001-973887	20010917
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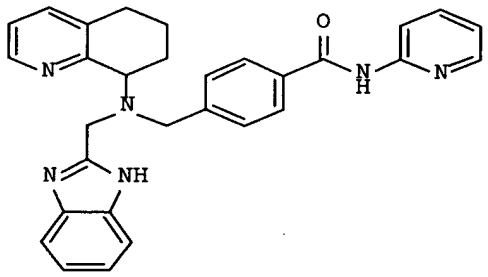
BR 2001013931	A	20040113	BR 2001-13931	20010917
JP 2004508421	T2	20040318	JP 2002-526852	20010917
NZ 524421	A	20050225	NZ 2001-524421	20010917
RU 2277092	C2	20060527	RU 2003-110578	20010917
AT 335733	E	20060915	AT 2001-975290	20010917
ZA 2003001399	A	20041122	ZA 2003-1399	20030220
NO 2003001178	A	20030314	NO 2003-1178	20030314
US 2004171638	A1	20040902	US 2004-799386	20040311
US 7091217	B2	20060815		
US 2005026942	A1	20050203	US 2004-914663	20040809
PRIORITY APPLN. INFO.:			US 2000-233087P	P 20000915
			US 2000-234816P	P 20000922
			US 2000-232891P	P 20000915
			US 2000-234510P	P 20000922
			US 2001-957654	A3 20010917
			WO 2001-CA1325	W 20010917
			US 2002-31812	A1 20020328

OTHER SOURCE(S): MARPAT 136:263159

GI



II

AB Members of a class of (mostly tertiary) amines, containing a multiplicity of heteroarom. substituents, and the salts and prodrug forms thereof, are useful as ***chemokine*** receptor modulators. In particular, compds. of formula X-L1-N(Z)-(CR12)n-Ar-L2-N(R2)-L3-Y (I) are disclosed [wherein: X = monocyclic (5-6 membered) or fused bicyclic (9-12 membered) (un)substituted ring system containing at least 1 N, O, or S atom; Z = H, monocyclic (5-6 membered) or fused bicyclic (9-12 membered) (un)substituted ring system containing at least 1 N, O, or S atom; Ar = (un)substituted aromatic or heteroarom. ring; each of

L1, L2, and L3 = bond, CO, SO2, or CH2, wherein at least 1 of L2 and L3 must comprise CO or SO2, and wherein L1 can also be alkylene (2-5C) wherein 1 or 2 C may optionally be replaced by N and which alkylene may itself optionally be substituted by a bridge alkylene (3-4C); L2 and L3 also may be, independently, SO2NH, CONH, SO2NHCH2 or CONHCH2; n = 0, 1, or 2; each R1 and R2 = H, straight or branched chain or cyclic alkyl (1-6C) which may optionally be substituted, and wherein R2 may be alkylene coupled to Y; and Y comprises at least 1 aromatic or heteroarom. or other heterocyclic (un)substituted ring coupled directly to L3]. The compds. are useful for treatment of conditions which are modulated by the ***chemokine*** receptors CXCR4 and CCR5, and particularly for treatment of patients infected with HIV or FIV. Examples include 54 syntheses and 3 bioassays, and many addnl. compds. within the invention are listed. For instance, amidation of 4-(chloromethyl)benzoyl chloride with 2-aminopyridine (49%), followed by amination of the chloride with 8-[N-(2-nitrobenzenesulfonyl)amino]-5,6,7,8-tetrahydroquinoline (92%), removal of the 2-nitrobenzenesulfonyl group from the amine using PhSH and K2CO3 in DMF (93%), and finally N-alkylation of the amine with N-BOC-2-(chloromethyl)benzimidazole and deprotection (47%), gave title compound II, designated AMD 9370. In a test for inhibition of Ca flux induced by the ***chemokine*** SDF-1α in SUP-T1 cells in vitro, 6 compds. including II gave > 20% inhibition at 20 μg/mL. In a test for inhibition of NL4.3/IIIB (CXCR4-using) HIV-1 in MT-4 cells in vitro, 7 compds. including II exhibited EC50 values < 20 μg/mL. The compds. also inhibited BaL (CCR5-using) HIV-1 similarly.

L32 ANSWER 27 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:	2001:765615 HCAPLUS Full-text
DOCUMENT NUMBER:	136:95768
TITLE:	AMD3100, a potent and specific antagonist of the stromal cell-derived factor-1 ***chemokine*** receptor CXCR4, inhibits autoimmune joint inflammation in IFN-γ receptor-deficient mice
AUTHOR(S):	Matthys, Patrick; Hatse, Sigrid; Vermeire, Kurt; Wuyts, Anja; ***Bridger, Gary***; Henson, Geoffrey W.; De Clercq, Erik; Billiau, Alfons; ***Schols, Dominique***
CORPORATE SOURCE:	Laboratories of Immunobiology, Rega Institute for Medical Research, Katholieke Universiteit Leuven, Louvain, B-3000, Belg.
SOURCE:	Journal of Immunology (2001), 167(8), 4686-4692 CODEN: JOIMA3; ISSN: 0022-1767
PUBLISHER:	American Association of Immunologists
DOCUMENT TYPE:	Journal
LANGUAGE:	English

AB Autoimmune collagen-induced arthritis (CIA) in IFN-γR-deficient DBA/1 mice was shown to be reduced in severity by treatment with the bicyclam derivative AMD3100, a specific antagonist of the interaction between the ***chemokine*** stromal cell-derived factor-1 (SDF-1) and its receptor CXCR4. The beneficial effect of the CXCR4 antagonist was demonstrable when treatment was initiated between the time of immunization and appearance of the first symptoms. Treatment also reduced the delayed-type hypersensitivity response to the autoantigen, collagen type II. These observations are indicative of an action on a late event in the pathogenesis, such as ***chemokine***-mediated attraction of leukocytes toward joint tissues. The notion of SDF-1 involvement was further supported by the observation that exogenous SDF-1 injected in periarthritic tissue elicited an inflammatory response that could be inhibited by AMD3100. The majority of leukocytes harvested from inflamed joints of mice with CIA

were found to be Mac-1+ and CXCR4+, and AMD3100 was demonstrated to interfere specifically with chemotaxis and Ca2+ mobilization induced in vitro by SDF-1 on Mac-1+/CXCR4+ splenocytes. We conclude that SDF-1 plays a central role in the pathogenesis of murine CIA, by attracting Mac-1+/CXCR4+ cells to the inflamed joints.

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 28 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:464869 HCAPLUS Full-text
DOCUMENT NUMBER: 135:266685
TITLE: Mutation of Asp171 and Asp262 of the ***chemokine*** receptor CXCR4 impairs its coreceptor function for human immunodeficiency virus-1 entry and abrogates the antagonistic activity of AMD3100
AUTHOR(S): Hatse, Sigrid; Princen, Katrien; Gerlach, Lars-Ole; ***Bridger, Gary***; Henson, Geoffrey; De Clercq, Erik; Schwartz, Thue W.; ***Schols, Dominique***
CORPORATE SOURCE: Rega Institute for Medical Research, Katholieke Universiteit Leuven, Louvain, Belg.
SOURCE: Molecular Pharmacology (2001), 60(1), 164-173
CODEN: MOPMA3; ISSN: 0026-895X
PUBLISHER: American Society for Pharmacology and Experimental Therapeutics
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The bicyclam AMD3100 is a highly potent and selective CXCR4 antagonist with strong antiviral activity against human immunodeficiency virus (HIV)-1 and HIV-2, which use CXCR4 as coreceptor for host cell entry. Here, the authors investigated the interaction of AMD3100 with CXCR4 at the mol. level by mutational anal. The authors established a set of stably transfected U87.CD4 cell lines expressing different mutant forms of CXCR4 (i.e., CXCR4[WT], CXCR4[D171N], CXCR4[D262N], CXCR4[D171N,D262N], and CXCR4[H281A]), to compare the activity of the compound against mutated vs. wild-type CXCR4. The authors found that the antagonistic action of AMD3100 against CXCR4 -as assessed by the inhibitory effects of the compound on stromal cell-derived factor (SDF-1) binding to its receptor and on SDF-1-induced intracellular Ca signaling, and by displacement of the CXCR4-specific antibody, clone 12G5- was greatly reduced by substitution of Asp171 and/or Asp262 by neutral asparagine residue(s). Both aspartates, but most particularly Asp262, also proved essential for the anti-HIV-1 activity of AMD3100 against the viruses NL4.3, IIIB, and HE. In contrast, substitution of His281 by a neutral Ala potentiated the antagonistic and antiviral effects of the compound in the different assay systems. Importantly, compared with the wild-type receptor, CXCR4[D262N] was much less effective, whereas CXCR4[D171N,D262N] completely failed as a coreceptor for infection by HIV-1 NL4.3. Thus, the neg. charged Asp residues at positions 171 and 262, located in transmembrane domains 4 and 6 of the 7-transmembrane receptor, resp., may represent crucial sites for electrostatic interaction of the pos. charges of the bicyclams, as well as for the highly basic V3 loop of the gp120 envelope protein of certain HIV-1 strains.

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 29 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:453052 HCAPLUS Full-text
DOCUMENT NUMBER: 135:46212
TITLE: ***Chemokine*** receptor binding heterocyclic compounds

INVENTOR(S): ***Bridger, Gary J.***; Boehringer, Eva Maria; Wang, Zhongren; ***Schols, Dominique***; ***Skerlj, Renato T.***; Bogucki, David E.
PATENT ASSIGNEE(S): Anormed Inc., Can.
SOURCE: PCT Int. Appl., 60 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001044229	A1	20010621	WO 2000-CA1503	20001215
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW				
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EP 1244648	A1	20021002	EP 2000-986914	20001215
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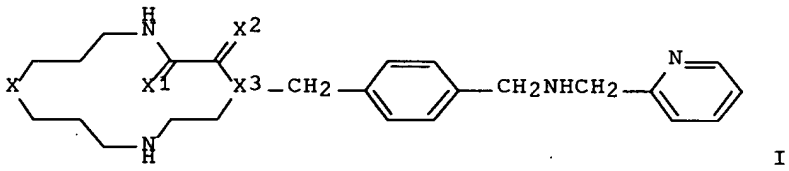
JP 2003516984	T2	20030520	JP 2001-544719	20001215
PRIORITY APPLN. INFO.:			US 1999-172153P	P 19991217
			WO 2000-CA1503	W 20001215

OTHER SOURCE(S): MARPAT 135:46212
GI



I

AB Monocyclic polyamines I [X = CHF, CF2, O, S, SO, SO2, X1, X2 = H2, X3 = N; X = CH2, X1 = O, X2 = H2, X3 = N; X = CH2, X1 = H2, X2 = O, X3 = N; X = O, X1, X2 = H2, X = CH] were prepared and have activity in standard tests against HIV- or FIV- infected cells as well as other biol. activity related to binding of ligands to ***chemokine*** receptors that mediate a number of mammalian embryonic developmental processes. Thus, I [X = N, X1, X2 = H2, X3 = N] was prepared from FCH[(CH2)3OTs]2 and (2- O2NC6H4SO2NHCH2CH2)2NP(O)(OEt)2 to form the macrocycle which was deblocked and treated with the N-protected bromide of the side chain, followed by deblocking.

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 30 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:329830 HCAPLUS Full-text
DOCUMENT NUMBER: 135:131824
TITLE: Molecular interactions of cyclam and bicyclam non-peptide antagonists with the CXCR4 ***chemokine*** receptor
AUTHOR(S): Gerlach, Lars Ole; ***Skerlj, Renato T.***; ***Bridger, Gary J.***; Schwartz, Thue W.
CORPORATE SOURCE: Laboratory for Molecular Pharmacology, Panum Institute, University of Copenhagen, Copenhagen, DK-2200, Den.
SOURCE: Journal of Biological Chemistry (2001), 276(17), 14153-14160
CODEN: JBCHA3; ISSN: 0021-9258
PUBLISHER: American Society for Biochemistry and Molecular Biology
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The non-peptide CXCR4 receptor antagonist AMD3100, which is a potent blocker of human immunodeficiency virus cell entry, is a sym. bicyclam composed of two identical 1,4,8,11-tetraazacyclotetradecane (cyclam) moieties connected by a relatively rigid phenylenebismethylene linker. Based on the known strong propensity of the cyclam moiety to bind carboxylic acid groups, receptor mutagenesis identified Asp171 and Asp262, located in transmembrane domain (TM) IV and TM-VI, resp., at each end of the main ligand-binding crevice of the CXCR4 receptor, as being essential for the ability of AMD3100 to block the binding of the ***chemokine*** ligand stromal cell-derived factor (SDF)-1α as well as the binding of the receptor antibody 12G5. The free cyclam moiety had no effect on 12G5 binding, but blocked SDF-1α binding with an affinity of 3 μM through interaction with Asp171. The effect on SDF-1α binding of a series of bicyclam analogs with variable chemical linkers was found to rely either only on Asp171, i.e. the bicyclams acted as the isolated cyclam, or on both Asp171 and Asp262, i.e. they acted as AMD3100, depending on the length and the chemical nature of the linker between the two cyclam moieties. A pos. correlation was found between the dependence of these compds. on Asp262 for binding and their potency as anti-human immunodeficiency virus agents. It is concluded that AMD3100 acts on the CXCR4 receptor through binding to Asp171 in TM-IV and Asp262 in TM-VI with each of its cyclam moieties, and it is suggested that part of its function is associated with a conformational constraint imposed upon the receptor by the connecting phenylene-bismethylene linker.

REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 31 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:201919 HCAPLUS Full-text
TITLE: CXCR4 receptor antagonist, AMD3100, is a potent inhibitor of HIV infection
AUTHOR(S): De Clercq, E.; ***Schols, D.***; ***Bridger, G.***; Henson, G.
CORPORATE SOURCE: Laboratory of Experimental Chemotherapy, Rega Institute for Medical Research, Louvain, Belg.
SOURCE: Abstracts of Papers, 221st ACS National Meeting, San Diego, CA, United States, April 1-5, 2001 (2001) MEDI-024
CODEN: 69FZD4
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal; Meeting Abstract
LANGUAGE: English

AB AMD3100, 1,1'-[1,4-phenylenebis-(methylene)]-bis-1,4,8,11-tetraazacyclotetradecane, is the prototype compound of the bicyclams and has been shown to interact specifically with the CXC-***chemokine*** receptor, CXCR4, the main coreceptor used by T-tropic (X4) HIV strains to enter their target cells. AMD3100 consistently blocks the replication of all X4 HIV and dual-tropic (R5/X4) variants that use CXCR4 for entering the cells (e.g T cell lines, CXCR4-transfected cell lines, lymphocytes and monocytes/macrophages). Against R5/X4 HIV-1 clin. isolates AMD3100 showed varying activity, depending on the clin. isolate, but the viruses that could be recovered from the AMD3100-treated cell cultures were unable to use CXCR4 and had lost their pathogenic SI phenotype. The anti-HIV potency of the bicyclams closely correlated with their potency in inhibiting the binding of anti-CXCR4 mAb (12G5) and inhibiting the binding and Ca2+ signaling of the natural ligand of CXCR4, SDF-1. AMD3100 had no signaling effect by itself and did not affect Ca2+ mobilization induced by any other CC or CXC-***chemokine*** evaluated so far. Also, in vivo in SCID-hu thy/liv and SCID-hu PBMC mice, AMD3100 was effective in preventing the replication of X4 HIV-1 clin. isolates. AMD3100 has been selected as the clin. drug candidate, which, after initial phase I (safety) studies, has proceeded to phase II (efficacy) trials.

L32 ANSWER 32 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:688234 HCAPLUS Full-text
DOCUMENT NUMBER: 133:266589
TITLE: Preparation of heterocyclic derivatives as ***chemokine*** receptor antagonists effective against HIV, tumor, and allergy
INVENTOR(S): ***Bridger, Gary***; ***Skerlj, Renato***; Kaller, Al; Harwig, Curtis; Bogucki, David; Wilson, Trevor R.; Crawford, Jason; ***McEachern, Ernest J.***; Atsma, Bem; Nan, Siqiao; Zhou, Yuanxi; ***Schols, Dominique***
PATENT ASSIGNEE(S): Anormed Inc., Can.
SOURCE: PCT Int. Appl., 274 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000056729	A1	20000928	WO 2000-CA321	20000324
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2368047	AA	20000928	CA 2000-2368047	20000324
EP 1163238	A1	20011219	EP 2000-913979	20000324
EP 1163238	B1	20060531		
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BR 2000010655	A	20020213	BR 2000-10655		20000324
TR 200102799	T2	20020722	TR 2001-2799		20000324
NZ 514709	A	20030328	NZ 2000-514709		20000324
JP 2003524620	T2	20030819	JP 2000-606590		20000324
US 6750348	B1	20040615	US 2000-535314		20000324
AU 775123	B2	20040715	AU 2000-35460		20000324
AT 327988	E	20060615	AT 2000-913979		20000324
NO 2001004593	A	20011029	NO 2001-4593		20010921
US 2004235823	A1	20041125	US 2004-837467		20040430
PRIORITY APPLN. INFO.:			US 1999-125823P	P	19990324
			US 2000-535314	A3	20000324
			WO 2000-CA321	W	20000324

OTHER SOURCE(S): MARPAT 133:266589

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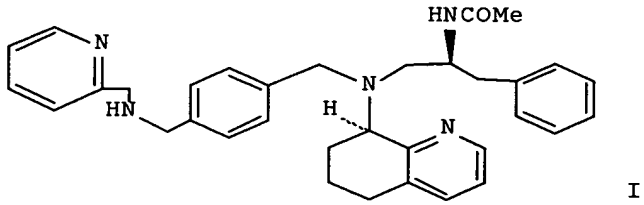

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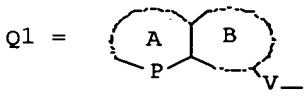

AB Title compds. [YW(X)(Z)(CR1R2)nArCR3R4N(R5)(CR6R7)qR8; W = N, Y is void; WY = CH; R1 to R7 may be the same or different and are independently selected from H, straight, branched or cyclic C1-6 alkyl; R8 = substituted heterocyclic group or a substituted aromatic group; Ar = aromatic or heteroarom. ring each optionally substituted at single or multiple, non-linking positions with electron-donating or withdrawing groups; n and q are independently = 0-2; X = Q, Q1; A = optionally substituted, saturated or unsatd. 5 or 6-membered ring; P = optionally substituted carbon atom, optionally substituted nitrogen atom, sulfur or oxygen atom; B = optionally substituted 5 to 7-membered ring; Ring A and Ring B in the above formula can be connected to the group W from any position via the group V; V = bond, (CH2)m, CO; m = 0-2; Z = H, optionally substituted C1-6 alkyl group, C0-6 alkyl group substituted with an optionally substituted aromatic or heterocyclic group, optionally substituted C0-6 alkylamino, C3-7 cycloalkylamino group, optionally substituted carbonyl group or sulfonyl], pharmaceutically acceptable acid addition, salts, metal complexes, stereoisomers, isomer mixts., and pharmaceutical composition are prepared Title compds. are having protective effects against infection by HIV through binding to ***chemokine*** receptors, including CXCR4 and CCR5 and inhibiting the subsequent binding of their natural ligands. Thus, the title

compound I was prepared and tested for inhibition of HIV-1 NL4.3 or IIIB replication in MT-4 cells and exhibited EC50's of less than 20μg/mL.

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 33 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:331726 HCAPLUS Full-text
TITLE: Synthesis and structure-activity relationships of bis-azamacrocycles that inhibit HIV-1 and HIV-2 replication by antagonism of the ***chemokine*** receptor CXCR4.
AUTHOR(S): ***Skerlj, Renato T.; Bridger, Gary J.*** ; Pabmanabhan, Screenivasan; Martellucci, Stephen A.; Henson, Geoffrey W.; Struyf, Sofie; Witvrouw, Myriam; ***Schols, Dominique***; De Clercq, Erik
CORPORATE SOURCE: AnorMED Inc, Langley, BC, V2N 1N5, Can.
SOURCE: Book of Abstracts, 219th ACS National Meeting, San Francisco, CA, March 26-30, 2000 (2000), MEDI-122. American Chemical Society: Washington, D. C.
CODEN: 69CLAC
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English

AB The bicyclam AMD3100 is a potent and selective inhibitor of HIV-1 and HIV-2 virus replication by binding to the ***chemokine*** receptor CXCR4, the co-receptor for X4 viruses. With the aim of optimizing the anti-HIV activity of bis-azamacrocycles, a series of compds. in which the secondary amine groups of AMD3100 were replaced by neutral heteroatom or heteroarom. groups were synthesized and evaluated for their inhibitory effects on HIV-1 and HIV-2 replication in vitro. It was found that the p-phenylenebis(methylene)-linked dimer of the py[iso-14]aneN4 (AMD3329) displayed the highest antiviral activity of the bis-azamacrocyclic analogs reported to date, exhibiting EC50's against the cytopathic effects of HIV-1 and HIV-2 of 0.8 and 1.6 nM, resp. AMD3329 also inhibited the binding of a specific CXCR4 mAb and Ca2+ flux induced by SDF-1α, the natural ligand for CXCR4, more potently than AMD3100 and also interfered with virus-induced syncytium formation at an EC50 of 12 nM.

L32 ANSWER 34 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:53607 HCAPLUS Full-text
DOCUMENT NUMBER: 132:107964
TITLE: Preparation of antiviral macrocyclic polyamines
INVENTOR(S): ***Bridger, Gary James***; Boehringer, Eva Maria; Wang, Zhongren; ***Schols, Dominique***; ***Skerlj, Renato Tony***; Bogucki, David Earl
PATENT ASSIGNEE(S): Anormed Inc., Can.
SOURCE: PCT Int. Appl., 69 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000002870	A1	20000120	WO 1999-CA619	19990708

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS,

JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

US 6506770	B1	20030114	US 1998-111895	19980708
CA 2336634	AA	20000120	CA 1999-2336634	19990708
AU 9945959	A1	20000201	AU 1999-45959	19990708
AU 767359	B2	20031106		
BR 9912524	A	20010502	BR 1999-12524	19990708
EP 1095031	A1	20010502	EP 1999-928956	19990708
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002520323	T2	20020709	JP 2000-559101	19990708
NZ 509699	A	20031031	NZ 1999-509699	19990708
NO 2001000047	A	20010301	NO 2001-47	20010104
US 6872714	B1	20050329	US 2001-743561	20010813
US 2005154005	A1	20050714	US 2004-991944	20041117
PRIORITY APPLN. INFO.:			US 1998-111895 A	19980708
			US 1996-659500 A2	19960606
			WO 1999-CA619 W	19990708
			US 2001-743561 A1	20010813

OTHER SOURCE(S): MARPAT 132:107964

AB Monocyclic polyamines V-CR1R2-Ar-CR3R4-NR5-(CR6R7)x-R8 (V = cyclic polyamine having a total of 9-24 members; R1-R7 = H, alkyl; R8 = heterocyclic group, aromatic group, SH; Ar = aromatic or heteroarom. ring; x = 1, 2) which have activity in standard tests against HIV- or FIV-infected cells as well as other biol. activity related to binding of ligands to ***chemokine*** receptors, were prepared E.g., N-[1,4,8,11- tetraazacyclotetradecanyl-1,4-phenylenebis(methylene)]-2- (aminomethyl)pyridine hexahydrobromide was prepared

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 35 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:538987 HCAPLUS Full-text
DOCUMENT NUMBER: 131:306743
TITLE: Synthesis and Structure-Activity Relationships of Phenylenebis(methylene)- Linked Bis-azamacrocycles That Inhibit HIV-1 and HIV-2 Replication by Antagonism of the ***Chemokine*** Receptor CXCR4
AUTHOR(S): ***Bridger, Gary J.***; ***Skerlj, Renato T.***; Padmanabhan, Sreenivasan; Martellucci, Stephen A.; Henson, Geoffrey W.; Struyf, Sofie; Witvrouw, Myriam; ***Schols, Dominique***; De Clercq, Erik
CORPORATE SOURCE: AnorMED Inc., Langley, BC, V2Y 1N5, Can.
SOURCE: Journal of Medicinal Chemistry (1999), 42(19), 3971-3981
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Bis-tetraazamacrocycles such as the bicyclam AMD3100 are a class of potent and selective anti-HIV-1 and HIV-2 agents that inhibit virus replication by binding to the ***chemokine*** receptor CXCR4, the co-receptor for entry of X4 viruses. With the aim of optimizing the anti-HIV-1 and HIV-2 activity of bis-azamacrocycles, a series of analogs were synthesized which contain neutral

heteroatom (oxygen, sulfur) or heteroarom. (of lower pKa than a secondary amine) replacements for the amino groups of AMD3100. The introduction of one or more heteroatoms such as oxygen or sulfur into the macrocyclic ring of p-phenylenebis(methylene)-linked dimers (to give N3X or N2X2 bis-macrocycles) gave analogs with substantially reduced anti-HIV-1 (IIIB) and anti-HIV-2 (ROD) potency. In addition, the bis-sulfur analog was also markedly more cytotoxic to MT-4 cells. However, bis-tetraazamacrocycles featuring a single pyridine group incorporated within the macrocyclic framework exhibited anti-HIV-1 and HIV-2 potency comparable to that of their saturated, aliphatic counterparts. The p-phenylenebis(methylene)-linked dimer of the py[14]aneN4 macrocycle inhibited HIV-1 replication at a 50% effective concentration (EC50) of 0.5 μM while remaining nontoxic to MT-4 cells at concns. approaching 200 μM. A series of analogs containing macrocyclic heteroarom. groups of varying pKa were also synthesized, and their ability to inhibit HIV replication was evaluated. Replacing the pyridine moiety of the py[14]aneN4 macrocyclic ring with pyrazine or pyridine groups substituted in the 4-position (with electron-withdrawing or -donating groups) either reduced antiviral potency or increased cytotoxicity to MT-4 cells. Finally, we synthesized a series of analogs in which the ring size of the bis-pyridyl macrocycles was varied between 12 and 16 members per ring including the py[iso-14]aneN4 ring system, an isomer of the py[14]aneN4 macrocycle. The p-phenylenebis(methylene)-linked dimer of the py[iso-14]aneN4 (AMD3329) displayed the highest antiviral activity of the bis-azamacrocyclic analogs reported to date, exhibiting EC50's against the cytopathic effects of HIV-1 and HIV-2 replication of 0.8 and 1.6 nM, resp., i.e., about 3-5-fold lower than the EC50 of AMD3100. AMD3329 also inhibited the binding of a specific CXCR4 mAb and the Ca2+ flux induced by SDF-1α, the natural ligand for CXCR4, more potently than AMD3100. Furthermore, AMD3329 also interfered with virus-induced syncytium formation at an EC50 of 12 nM.

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 36 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:456438 HCAPLUS Full-text
DOCUMENT NUMBER: 131:223050
TITLE: Bicyclams, selective antagonists of the human ***chemokine*** receptor CXCR4, potently inhibit feline immunodeficiency virus replication
AUTHOR(S): Egberink, Herman F.; De Clercq, Erik; Van Vliet, Arno L. W.; Balzarini, Jan; ***Bridger, Gary J.***; Henson, Geoffrey; Horzinek, Marian C.; ***Schols, Dominique***
CORPORATE SOURCE: Institute of Virology, Utrecht University, Utrecht, 3584 CL, Neth.
SOURCE: Journal of Virology (1999), 73(8), 6346-6352
CODEN: JOVIAM; ISSN: 0022-538X
PUBLISHER: American Society for Microbiology
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Bicyclams are low-mol.-weight anti-human immunodeficiency virus (HIV) agents that have been shown to act as potent and selective CXC ***chemokine*** receptor 4 (CXCR4) antagonists. Here, the authors demonstrate that bicyclams are potent inhibitors of feline immunodeficiency virus (FIV) replication when evaluated in Crandell feline kidney (CRFK) cells. With a series of bicyclam derivs., 50% inhibitory concns. (IC50s) against FIV were obtained in this cell system that were comparable to those obtained for HIV-1 IIIB replication in the human CD4+ MT-4 T-cell line. The bicyclams were also able to block FIV replication in feline thymocytes, albeit at higher concns. than in the CRFK cells. The

prototype bicyclam AMD3100, 1-1'-[1,4-phenylene-bis(methylene)]-bis(1,4,8,11-tetraazacyclotetradecane),was only fourfold less active in feline thymocytes (IC50, 62 ng/mL) than in CRFK cells (IC50, 14 ng/mL). AMD2763, 1,1'-propylene-bis(1,4,8,11-tetraazacyclotetradecane), which is a less potent CXCR4 antagonist, was virtually inactive against FIV in feline thymocytes (IC50, >66.5 μg/mL), while it was clearly active in CRFK cells (IC50, 0.9 μg/mL). The CXC ***chemokine*** stromal-cell-derived factor 1α had anti-FIV activity in CRFK cells (IC50, 200 ng/mL) but not in feline thymocytes (IC50, >2.5 μg/mL). When primary FIV isolates were evaluated for their drug susceptibility in feline thymocytes, the bicyclams AMD3100 and its Zn2+ complex, AMD3479, inhibited all six primary isolates at equal potency. The marked susceptibility of FIV to the bicyclams suggests that FIV predominantly uses feline CXCR4 for entering its target cells.

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 37 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:398720 HCAPLUS Full-text
DOCUMENT NUMBER: 131:179354
TITLE: Shift of clinical human immunodeficiency virus type 1 isolates from X4 to R5 and prevention of emergence of the syncytium-inducing phenotype by blockade of CXCR4
AUTHOR(S): Este, Jose A.; Cabrera, Cecilia; Blanco, Julia; Gutierrez, Arantxa; ***Bridger, Gary***; Henson, Geoffrey; Clotet, Bonaventura; ***Schols, Dominique***; De Clercq, Erik
CORPORATE SOURCE: Institut de Recerca de la SIDA-Caixa, Retrovirology Laboratory, Hospital Universitari Germans Trias i Pujol, Badalona, 08916, Spain
SOURCE: Journal of Virology (1999), 73(7), 5577-5585
CODEN: JOVIAM; ISSN: 0022-538X
PUBLISHER: American Society for Microbiology
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The emergence of X4 human immunodeficiency virus type 1 (HIV-1) strains in HIV-1-infected individuals has been associated with CD4+ T-cell depletion, HIV-mediated CD8+ cell apoptosis, and an impaired humoral response. The bicyclam AMD3100, a selective antagonist of CXCR4, selected for the outgrowth of R5 virus after cultivation of mixts. of the laboratory-adapted R5 (BaL) and X4 (NL4-3) HIV strains in the presence of the compound The addition of AMD3100 to peripheral blood mononuclear cells infected with X4 or R5X4 clin. HIV isolates displaying the syncytium-inducing phenotype resulted in a complete suppression of X4 variants and a concomitant genotypic change in the V2 and V3 loops of the envelope gp120 glycoprotein. The recovered viruses corresponded genotypically and phenotypically to R5 variants in that they could no longer use CXCR4 as coreceptor or induce syncytium formation in MT-2 cells. Furthermore, the phenotype and genotype of a cloned R5 HIV-1 virus converted to those of the R5X4 virus after prolonged culture in lymphoid cells. However, these changes did not occur when the infected cells were cultured in the presence of AMD3100, despite low levels of virus replication. Our findings indicate that selective blockade of the CXCR4 receptor prevents the switch from the less pathogenic R5 HIV to the more pathogenic X4 HIV strains, a process that heralds the onset of AIDS. In this article, we show that it could be possible to redirect the evolution of HIV so as to impede the emergence of X4 strains or to change the phenotype of already-existing X4 isolates to R5.

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 38 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:36649 HCAPLUS Full-text
DOCUMENT NUMBER: 130:246282
TITLE: Activity of different bicyclam derivatives against human immunodeficiency virus depends on their interaction with the CXCR4 ***chemokine*** receptor
AUTHOR(S): Este, Jose A.; Cabrera, Cecilia; De Clercq, Erik; Struyf, Sofie; Van Damme, Jo; ***Bridger, Gary***; ***Skerlj, Renato T.***; Abrams, Michael J.; Henson, Geoffrey; Gutierrez, Arantxa; Clotet, Bonaventura; ***Schols, Dominique***
CORPORATE SOURCE: Institut de la Recerca de la SIDA-Caixa, Retrovirology Laboratory, Hospital Universitari Germans Trias i Pujol, Badalona, Spain
SOURCE: Molecular Pharmacology (1999), 55(1), 67-73
CODEN: MOPMA3; ISSN: 0026-895X
PUBLISHER: American Society for Pharmacology and Experimental Therapeutics
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Bicyclams represent a novel class of selective anti-HIV inhibitors with potent activity against T-cell tropic strains of HIV. The prototype compound, the bicyclam AMD3100, has an EC50 of 1 to 10 ng/mL against different strains of HIV-1, including clin. isolates. AMD3100 was shown to interact with the CXC-***chemokine*** receptor CXCR4, the main coreceptor used by T-cell tropic strains of HIV. Here the authors describe the interaction of different bicyclam derivs. with CXCR4. A close correlation ($r^2 = 0.7$) was found between the anti-HIV potency of the bicyclams and their ability to inhibit the binding of an anti-CXCR4 monoclonal antibody or the intracellular Ca++ signal induced by the stromal cell-derived factor-1α, the natural ligand of CXCR4. These results indicate that the mechanism of action of bicyclams is primarily mediated by their interaction with CXCR4. The most potent interaction with CXCR4 and thus anti-HIV activity was shown by bicyclam analogs with cyclam rings composed of fourteen members that are linked by an aromatic (phenyl) bridge. Elucidating the structural requirements for receptor interaction and the site(s) of interaction of bicyclams with CXCR4 will aid in the understanding of HIV-cell fusion.
REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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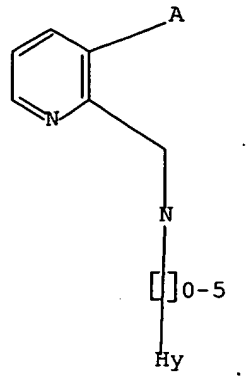

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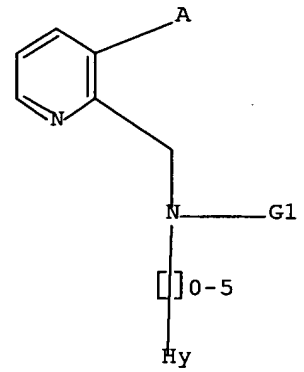

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L22 143 SEA FILE=HCAPLUS ABB=ON PLU=ON ("BRIDGER G"/AU OR "BRIDGER G J"/AU OR "BRIDGER G L"/AU OR "BRIDGER G M"/AU OR "BRIDGER G P"/AU OR "BRIDGER G W"/AU OR "BRIDGER GARY"/AU OR "BRIDGER GARY J"/AU OR "BRIDGER GARY JAMES"/AU)
L23 27 SEA FILE=HCAPLUS ABB=ON PLU=ON ("MCEACHERN E"/AU OR "MCEACHER N E J"/AU OR "MCEACHERN ERNEST"/AU OR "MCEACHERN ERNEST J"/AU OR "MCEACHERN ERNEST JOHN"/AU OR "MCEACHERN ERNIE J"/AU)
L24 68 SEA FILE=HCAPLUS ABB=ON PLU=ON ("SKERLJ R"/AU OR "SKERLJ R T"/AU OR "SKERLJ RENATO"/AU OR "SKERLJ RENATO T"/AU OR "SKERLJ RENATO TONY"/AU)
L25 205 SEA FILE=HCAPLUS ABB=ON PLU=ON ("SCHOLS D"/AU OR "SCHOLS DOMINIQUE"/AU OR "SCHOLS DOMINQUE"/AU)
L26 52 SEA FILE=HCAPLUS ABB=ON PLU=ON (L22 AND (L23 OR L24 OR L25)) OR (L23 AND (L24 OR L25)) OR (L24 AND L25)

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L27          52 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L22 AND (L23 OR L24 OR L25))

L28          12 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L23 AND (L24 OR L25))
L29          19 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L24 AND L25
L30          23 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L27 AND (L28 OR L29)) OR
                (L28 AND L29)
L31          34 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L26 AND (?CHEMOKINE?)
L32          38 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L31 OR L30)
L36          34 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L19 NOT L32


=> d ibib abs hitstr l36 tot

L36  ANSWER 1 OF 34  HCAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:         2006:707358  HCAPLUS  Full-text
DOCUMENT NUMBER:          145:145555
TITLE:                    Preparation of aryl and heteroaryl sulfonamides as
                          CCR2 antagonists
INVENTOR(S):              Ungashe, Solomon
PATENT ASSIGNEE(S):       Chemocentryx, Inc., USA
SOURCE:                   PCT Int. Appl., 270 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.          DATE
     ---------------      ----   --------    --------------------     --------
     WO 2006076644         A2    20060720    WO 2006-US1341           20060113
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR,
             KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX,
             MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE,
             SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC,
             VN, YU, ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
     US 2006173019         A1    20060803    US 2006-332786           20060113
PRIORITY APPLN. INFO.:                       US 2005-644103P      P   20050114
                                             US 2005-742821P      P   20051206
                                             US 2005-750985P      P   20051216
OTHER SOURCE(S):          MARPAT 145:145555
GI
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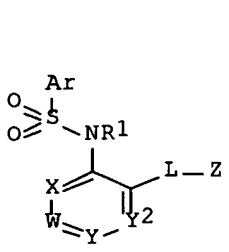

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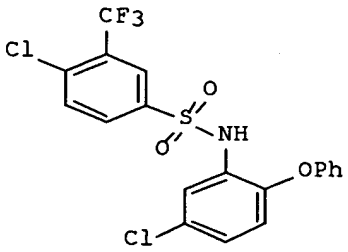


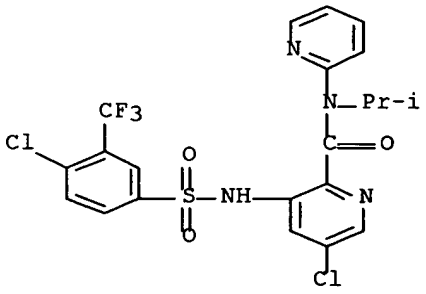
II

AB Title compds. I [Ar = (un)substituted aryl or heteroaryl; R1 = H, (un)substituted alkyl, alkenyl, etc.; X, W, and Y independently = CR2, N, and N(=O), where each occurrence of R2 independently = CN, CHO, CO2H, alkylcarbonyl, etc.; Y2 = N or N(=O); L = bond, O, S, SO, etc.; Z = (un)substituted aryl, heteroaryl, heterocyclyl, etc.], are prepared and disclosed as potent antagonists of the CCR2 receptor. Thus, e.g., II was prepared by reaction of 5-chloro-2-phenoxyphenylamine with 4-chloro-3-trifluoromethylbenzenesulfonyl chloride. Numerous compds. of the invention demonstrated IC50 values < 500 nM in assays for CCR2 activity. Animal testing demonstrates that these compds. are useful for treating inflammation, a hallmark disease for CCR2. The compds. are generally aryl sulfonamide derivs. and are useful in pharmaceutical compns., methods for the treatment of CCR2-mediated diseases, and as controls in assays for the identification of CCR2 antagonists.

IT ***899423-21-3P 899423-29-1P 899423-34-8P 899423-40-6P 899423-41-7P 899423-42-8P***
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heteroaryl sulfonamides as CCR2 receptor antagonists)

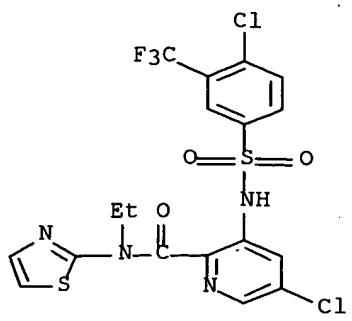
RN 899423-21-3 HCAPLUS

CN 2-Pyridinecarboxamide, 5-chloro-3-[[[4-chloro-3-(trifluoromethyl)phenyl]sulfonyl]amino]-N-(1-methylethyl)-N-2-pyridinyl- (9CI) (CA INDEX NAME)

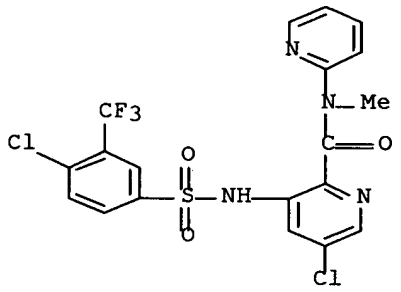


RN 899423-29-1 HCAPLUS

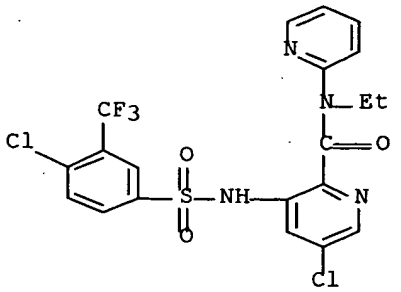
CN 2-Pyridinecarboxamide, 5-chloro-3-[[[4-chloro-3-(trifluoromethyl)phenyl]sulfonyl]amino]-N-ethyl-N-2-thiazolyl- (9CI) (CA INDEX NAME)



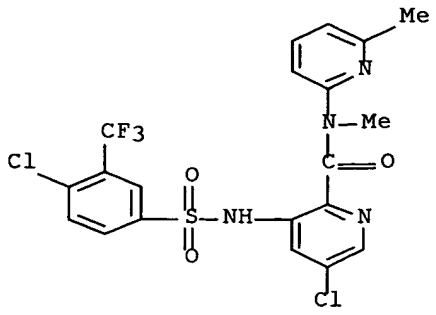
RN 899423-34-8 HCAPLUS
CN 2-Pyridinecarboxamide, 5-chloro-3-[[[4-chloro-3-(trifluoromethyl)phenyl]sulfonyl]amino]-N-methyl-N-2-pyridinyl- (9CI) (CA INDEX NAME)



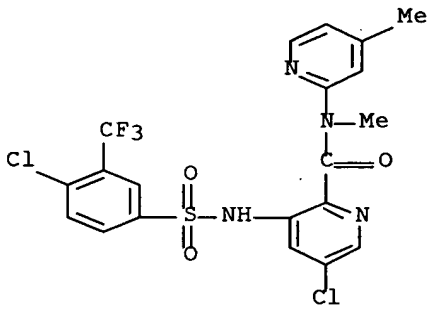
RN 899423-40-6 HCAPLUS
CN 2-Pyridinecarboxamide, 5-chloro-3-[[[4-chloro-3-(trifluoromethyl)phenyl]sulfonyl]amino]-N-ethyl-N-2-pyridinyl- (9CI) (CA INDEX NAME)



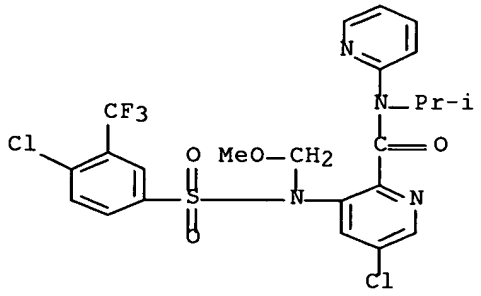
RN 899423-41-7 HCAPLUS
CN 2-Pyridinecarboxamide, 5-chloro-3-[[[4-chloro-3-(trifluoromethyl)phenyl]sulfonyl]amino]-N-methyl-N-(6-methyl-2-pyridinyl)-(9CI) (CA INDEX NAME)



RN 899423-42-8 HCAPLUS
CN 2-Pyridinecarboxamide, 5-chloro-3-[[[4-chloro-3-(trifluoromethyl)phenyl]sulfonyl]amino]-N-methyl-N-(4-methyl-2-pyridinyl)-(9CI) (CA INDEX NAME)



IT ***899424-56-7P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of heteroaryl sulfonamides as CCR2 receptor antagonists)
RN 899424-56-7 HCAPLUS
CN 2-Pyridinecarboxamide, 5-chloro-3-[[[4-chloro-3-(trifluoromethyl)phenyl]sulfonyl](methoxymethyl)amino]-N-(1-methylethyl)-N-2-pyridinyl- (9CI) (CA INDEX NAME)

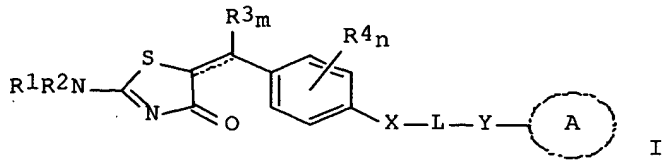


L36 ANSWER 2 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:411688 HCAPLUS Full-text
DOCUMENT NUMBER: 144:450700
TITLE: Preparation of benzylidene thiazolones as α-estrogen receptors modulators
INVENTOR(S): Martin, Richard; Mohan, Raju; Busch, Brett B.; Nyman, Michael Charles; Stevens, William C., Jr.
PATENT ASSIGNEE(S): Exelixis, Inc., USA
SOURCE: PCT Int. Appl., 135 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006047269	A2	20060504	WO 2005-US37853	20051021
WO 2006047269	A3	20060720		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2004-621296P P 20041022
OTHER SOURCE(S): MARPAT 144:450700
GI



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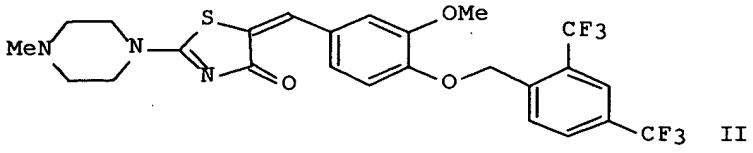


II

AB Title compds. represented by the formula I [wherein R1, R2 = independently (un)substituted (cyclo)alkyl, alkenyl, alkynyl, etc.; or R1R2N = (un)substituted heterocyclyl or heteroaryl; R3 = H, halo or (un)substituted alkyl; R4 = independently halo, cyano, (un)substituted alkyl, etc.; m = 1 or 2; n = 0-4; X, Y = independently O, NR8, SOp or a direct bond ; p = 0-2; R8 = H or (un)substituted alkyl; L = (un)substituted alkylene, cycloalkyl, alkenylene or alkynylene; A = (un)substituted (hetero)aryl; and pharmaceutically acceptable salts thereof] were prepared as α-estrogen receptors (ERRα) modulators. For example, II was provided in a multi-step synthesis starting from reaction of 1-bromomethyl-2,4-bis(trifluoromethyl)benzene with vanillin. II showed inverse agonist activity in the GAL4-ERRα assay with IC50 value of less than 0.5 μM and 100-120% control rate. Thus, I are useful for the treatment of ERRα related diseases,disorders or conditions, such as cancer (no data).

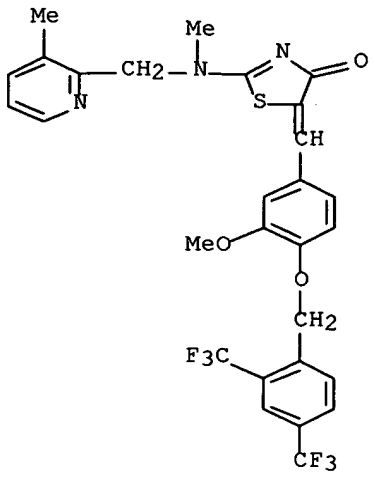
IT ***885599-03-1P***

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 5-benzylidene-4-thiazolone derivs. as α-estrogen receptors modulators)

RN 885599-03-1 HCAPLUS

CN 4(5H)-Thiazolone, 5-[[4-[[2,4-bis(trifluoromethyl)phenyl]methoxy]-3-methoxyphenyl]methylene]-2-[methyl[(3-methyl-2-pyridinyl)methyl]amino]-(9CI) (CA INDEX NAME)



L36 ANSWER 3 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:301786 HCAPLUS Full-text
DOCUMENT NUMBER: 144:331262
TITLE: 2-(Aminomethyl)indoles as histamine-3 receptor antagonists, their preparation, pharmaceutical compositions, and use in therapy
INVENTOR(S): Wager, Travis T.
PATENT ASSIGNEE(S): Pfizer Inc, USA
SOURCE: U.S. Pat. Appl. Publ., 26 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2006069087	A1	20060330	US 2005-224913	20050912
WO 2006035308	A1	20060406	WO 2005-IB2991	20050916

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2004-613796P P 20040927
GI

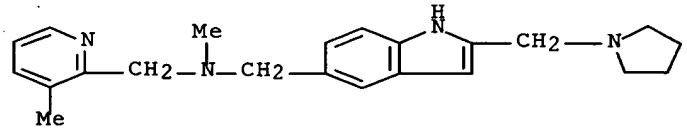
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to 2-(aminomethyl)indoles I, which are histamine-3 antagonists. In compds. I, R1 and R2 are independently selected from H, (un)substituted C1-8 alkyl, C3-7 cycloalkyl, 3- to 8-membered heterocyclyl, optionally substituted with C2-5 acyl, C6-10 arylsulfonyl, optionally substituted with Me or Et; and 5- to 10-membered heteroaryl, or R1 and R2, together with the adjacent nitrogen atom, form a 4- to 7-membered heterocyclyl ring; R3 is selected from optionally halo-substituted C1-8 alkyl, C3-7 cycloalkyl, and C6-14 aryl, or R1 and R3, together with the adjacent atoms, form a 4- to 7-membered heterocyclyl ring; R4 is H or optionally halo-substituted C1-8 alkyl; R5 is (un)substituted aminomethyl; each X is independently selected from halo, optionally fluoro-substituted C1-6 alkyl, optionally fluoro-substituted C1-6 alkoxy, and (un)substituted C1-6 alkyl-S(O)p, where p is 0, 1, or 2; and n is 0-3. The invention also relates to the preparation of I, pharmaceutical compns. comprising a compound I, optionally a pharmaceutically acceptable carrier, and optionally another therapeutic agent selected from H1 receptor antagonists and neurotransmitter re-uptake blockers, as well as to the use of the compns. for the treatment of a disorder or condition that may respond to antagonism of histamine-3 receptors. N-Acylation of Me 4-amino-3-iodobenzoate followed by coupling with propargyl alc. and cyclization gave (hydroxymethyl)indolecarboxylate II, which underwent oxidation, reductive amination with pyrrolidine, and hydride reduction to give (pyrrolidinylmethyl)indole III. Indole III was oxidized and aminated reductively with 1-acetylpiperazine resulting in the formation of indole IV. The compds. of the invention are antagonists of histamine-3 receptors (no data).

IT ***880361-02-4P***, Methyl-((3-methylpyridin-2-yl)methyl)-((2-((pyrrolidin-1-yl)methyl)-1H-indol-5-yl)methyl)amine
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of (aminomethyl)indoles as histamine-3 receptor antagonists)

RN 880361-02-4 HCAPLUS

CN 1H-Indole-5-methanamine, N-methyl-N-[(3-methyl-2-pyridinyl)methyl]-2-(1-pyrrolidinylmethyl)- (9CI) (CA INDEX NAME)



L36 ANSWER 4 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2006:292684 HCAPLUS Full-text

DOCUMENT NUMBER: 144:468150

TITLE: Preparation of thiazole derivatives as anti-infective agents

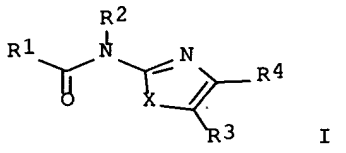
INVENTOR(S): Nan, Fajun; Li, Jia; Ye, Qizhuang

PATENT ASSIGNEE(S): Shang Medicine Inst., Chinese Academy of Sciences,

Peop. Rep. China
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 35 pp.
CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1580056	A	20050216	CN 2003-142277	20030815
PRIORITY APPLN. INFO.:			CN 2003-142277	20030815

GI



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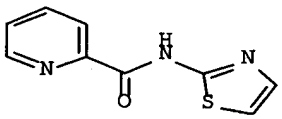


II

AB The title compds. I [wherein R1 = alkyl, alkenyl, alkynyl, etc.; R2 = alkyl, alkenyl, alkynyl, etc.; R3 = H, halo, alkyl, etc.; R4 = H, alkyl, cycloalkyl, etc.; X = O, S, or NH] are prepared as antiinfective agents for respiratory tract virus, enterovirus, hepatitis virus, pocky virus, herpes virus, and AIDS virus. For example, the compound II was prepared in a multi-step synthesis. Some of the compds. I showed good antiviral activities.

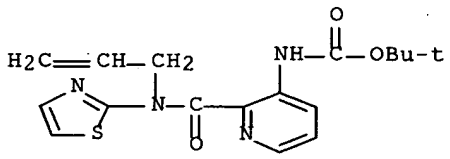
IT ***886467-13-6P 886467-23-8P 886467-24-9P***

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of thiazole derivs. as anti-infective agents)

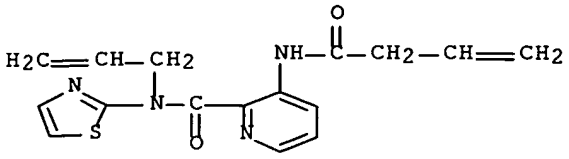
RN 886467-13-6 HCAPLUS

CN Carbamic acid, [2-[(2-propenyl-2-thiazolylamino)carbonyl]-3-pyridinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

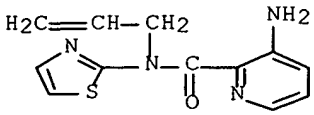


RN 886467-23-8 HCAPLUS

CN 2-Pyridinecarboxamide, 3-[(1-oxo-3-butenyl)amino]-N-2-propenyl-N-2-thiazolyl- (9CI) (CA INDEX NAME)



RN 886467-24-9 HCAPLUS
CN 2-Pyridinecarboxamide, 3-amino-N-2-propenyl-N-2-thiazolyl- (9CI) (CA INDEX NAME)

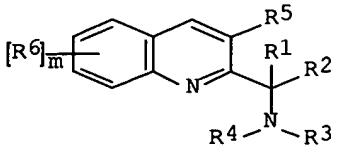


L36 ANSWER 5 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:1242837 HCAPLUS Full-text
DOCUMENT NUMBER: 144:6685
TITLE: Preparation of substituted quinolines for treating disorders mediated by KSP
INVENTOR(S): Wang, Weibo; Constantine, Ryan N.; Lagniton, Liana Marie; Bair, Kenneth
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 25 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005261337	A1	20051124	US 2005-133509	20050519
WO 2005113507	A1	20051201	WO 2005-US17961	20050519

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2004-573120P P 20040521
OTHER SOURCE(S): MARPAT 144:6685
GI



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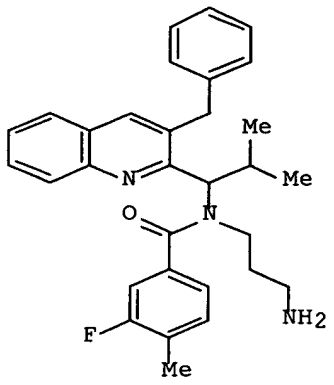


II

AB The title compds. I [m = 0-3; R1 = acylamino, carboxyl ester, and alkyl optionally substituted with OH or halo; R2 = H, alkyl; R3 = C(:X)A; A = (un)substituted aryl, heteroaryl, heterocyclyl, cycloalkyl; X = O, S; R4 = alkylene-heterocyclic or alkylene-NR7R8; R5 = L-A1; A1 = (un)substituted aryl, heteroaryl, heterocyclyl, cycloalkyl; L = O, NH, N(alkyl), etc.; R6 = alkyl, alkenyl, alkynyl, etc.; R7, R8 = H, alkyl, arylalkyl, etc.], useful for treating a disorder mediated, at least in part, by KSP in a mammalian patient, such as cancer, were prepared and formulated. E.g., a multi-step synthesis of II, starting from 2-chloro-3- (phenylmethyl)quinoline, was given. The preferred compds. I have a biol. activity as measured by an IC50 of less than about 1 μM in an assay for determining KSP activity.

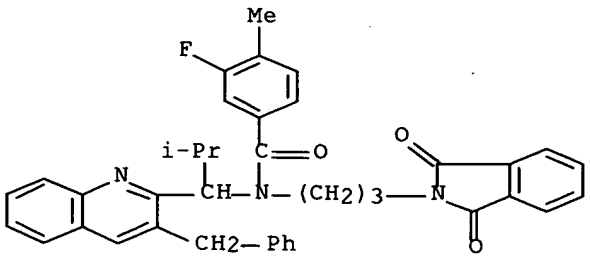
IT ***870070-67-0P***

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of substituted quinolines for treating disorders mediated by KSP)

RN 870070-67-0 HCAPLUS

CN Benzamide, N-[3-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)propyl]-3-fluoro-4-methyl-N-[2-methyl-1-[3-(phenylmethyl)-2-quinolinyl]propyl]- (9CI) (CA INDEX NAME)



L36 ANSWER 6 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:238977 HCAPLUS Full-text
DOCUMENT NUMBER: 142:298009
TITLE: A preparation of library of 4-piperidylcarboxamide derivatives capable of binding to a G-protein coupled receptor
INVENTOR(S): Jones, Graham Peter; MacRitchie, Jacqueline Anne; Slater, Martin John
PATENT ASSIGNEE(S): Biofocus PLC, UK
SOURCE: PCT Int. Appl., 51 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005023794	A2	20050317	WO 2004-GB3850	20040908
WO 2005023794	A3	20050602		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: GB 2003-20983 A 20030908
OTHER SOURCE(S): MARPAT 142:298009
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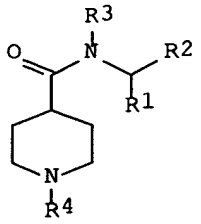

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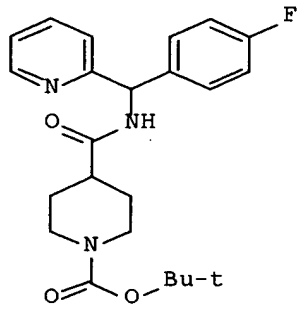

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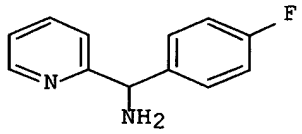


III

AB The invention relates to a preparation of library of 4-piperidylcarboxamide derivs. of formula I [wherein: R1 is derivs. of cyanopyridine, cyanopyrazine, cyanothiophene, or cyanopyrimidine, etc.; R2 is derivs. of 3-F-C6H4MgBr, 4-Me-C6H4MgBr, 4-Me2N-C6H4MgBr, or 4-Cl-C6H4MgBr, etc.; R3 is H or alkyl; R4 is acyl, sulfonyl, carbamoyl, or thiocarbamoyl, etc.] targeted to receptors that recognize a central secondary amide moiety and capable of binding to G-protein coupled receptor (no biol. data). The library was designed around an acetamide coupled to a piperidine moiety. A combination of specific motifs R1, R2, R3, and R4 were appended from the central scaffold and were designed to pick up different interactions at a receptor site. For instance, 4-piperidylcarboxamide derivative II was prepared via amidation of 1-(tert-butoxycarbonyl)piperidine-4-carboxylic acid by amine III.

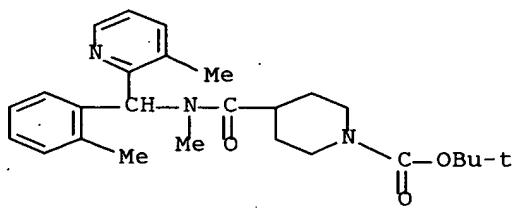
IT ***847923-57-3P***

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

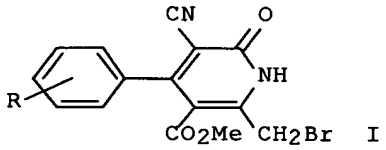
(preparation of library of 4-piperidylcarboxamide derivs. capable of binding to G-protein coupled receptor)

RN 847923-57-3 HCAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[methyl[(2-methylphenyl)(3-methyl-2-pyridinyl)methyl]amino]carbonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



L36 ANSWER 7 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:29841 HCAPLUS Full-text
DOCUMENT NUMBER: 143:7564
TITLE: Synthesis of 6-bromomethyl-substituted derivatives of pyridin-2(1H)-ones and their reaction with nucleophiles
AUTHOR(S): Kalme, Z. A.; Zhalubovskis, R. A.; Shmidlers, A.; Celmins, J.; Dubur, G.
CORPORATE SOURCE: Latvian Institute of Organic Synthesis, Riga, LV 1006, Latvia
SOURCE: Chemistry of Heterocyclic Compounds (New York, NY, United States)(Translation of Khimiya Geterotsiklicheskikh Soedinenii) (2004), 40(7), 862-868
CODEN: CHCCAL; ISSN: 0009-3122
PUBLISHER: Kluwer Academic/Consultants Bureau
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:7564
GI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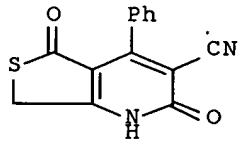
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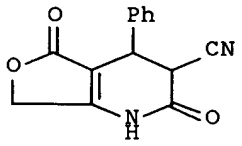
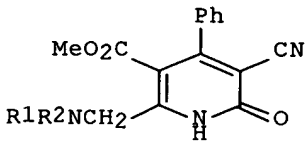
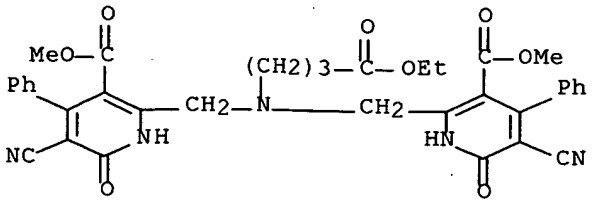

III


IV

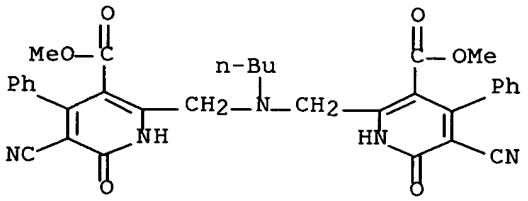
AB 6-Bromomethyl-substituted derivs. of pyridin-2(1H)-ones (I; R = H, 3-NO2, 4-NO2) were obtained by bromination of 6-methyl-3,4-dihydropyridin-2(1H)- ones and are the basis for the synthesis of thieno- (II) and furo[3,4-b]pyridin-2(1H)-ones (III) and also for obtaining new amino derivs. in the pyridin-2(1H)-one series, e.g., IV (R1R2N = piperidino, PhCH2CH2NH, PhNH, NHCH2COOEt).

IT ***852241-04-4P 852241-05-5P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of 6-bromomethyl-substituted derivs. of 2(1H)-pyridinones and their reaction with nucleophiles)

RN 852241-04-4 HCAPLUS
CN 3-Pyridinecarboxylic acid, 2,2'-[[(4-ethoxy-4-oxobutyl)imino]bis(methylene)]bis[5-cyano-1,6-dihydro-6-oxo-4-phenyl-, dimethyl ester (9CI) (CA INDEX NAME)



RN 852241-05-5 HCAPLUS
CN 3-Pyridinecarboxylic acid, 2,2'-[(butylimino)bis(methylene)]bis[5-cyano-1,6-dihydro-6-oxo-4-phenyl-, dimethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 8 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:14372 HCAPLUS Full-text
DOCUMENT NUMBER: 142:113884
TITLE: Preparation of 3-aminopyrrolidines as inhibitors of monoamine uptake
INVENTOR(S): Beadle, Christopher David; Cases-Thomas, Manuel Javier; Clark, Barry Peter; Gallagher, Peter Thaddeus; Masters, John Joseph; Timms, Graham Henry; Walter, Magnus Wilhelm; Whatton, Maria Ann; Wood, Virginia Ann; Gilmore, Jeremy
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 166 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005000811	A1	20050106	WO 2004-US13004	20040511

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1638934 A1 20060329 EP 2004-750759 20040511

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK

PRIORITY APPLN. INFO.:

GB 2003-13463	A	20030611
US 2003-510867P	P	20031014
US 2003-524450P	P	20031124
US 2003-524781P	P	20031125
WO 2004-US13004	W	20040511

OTHER SOURCE(S): MARPAT 142:113884

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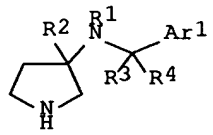


I

AB Title compds. [I; R1 = (substituted) alkyl, alkenyl, (CH2)qAr2, etc.; R2-R4 = H, alkyl; Ar1, Ar2 = (substituted) Ph, naphthyl, 5-6 membered heteroaryl; with provisos], were prepared Thus, tert-Bu (3S)-3-[(1-methylethyl)amino]pyrrolidine-1-carboxylate, 3,5-dichlorobenzaldehyde, and NaBH(OAc)3 were stirred 72 h in tri-Me orthoformate to give tert-Bu (3S)-3-[(1-methylethyl)-[[3,5- dichlorophenyl]methyl]amino]pyrrolidine-1-carboxylate. This was stirred 30 min. in CH2Cl2/CF3CO2H to give (3S)-N-(1-methylethyl)-N-[[3,5- dichlorophenyl]methyl]pyrrolidin-3-amine isolated as the D-tartrate. I showed Ki <200 nM for inhibition of reuptake of ≥1 of serotonin, norepinephrine, and dopamine by their transporter proteins.

IT ***820984-83-6P 820984-86-9P***

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of aminopyrrolidines as inhibitors of monoamine uptake)

RN 820984-83-6 HCAPLUS

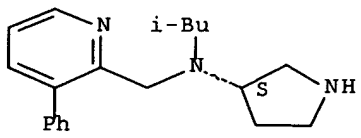
CN 2-Pyridinemethanamine, N-(2-methylpropyl)-3-phenyl-N-(3S)-3-pyrrolidinyl-, (2R,3R)-2,3-dihydroxybutanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 820984-82-5

CMF C20 H27 N3

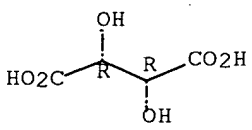
Absolute stereochemistry.



CM 2

CRN 87-69-4
CMF C4 H6 O6

Absolute stereochemistry.

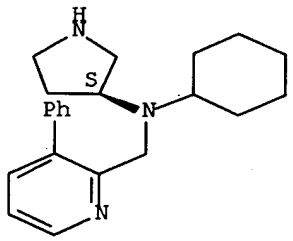


RN 820984-86-9 HCAPLUS
CN 2-Pyridinemethanamine, N-cyclohexyl-3-phenyl-N-(3S)-3-pyrrolidinyl-, (2R,3R)-2,3-dihydroxybutanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 820984-85-8
CMF C22 H29 N3

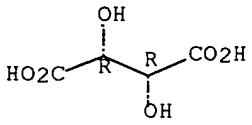
Absolute stereochemistry.



CM 2

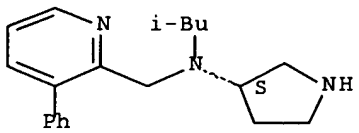
CRN 87-69-4
CMF C4 H6 O6

Absolute stereochemistry.



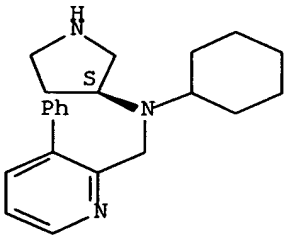
IT ***820984-82-5 820984-85-8***
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation of aminopyrrolidines as inhibitors of monoamine uptake)
RN 820984-82-5 HCAPLUS
CN 2-Pyridinemethanamine, N-(2-methylpropyl)-3-phenyl-N-(3S)-3-pyrrolidinyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



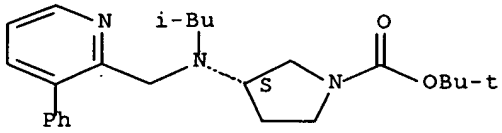
RN 820984-85-8 HCAPLUS
CN 2-Pyridinemethanamine, N-cyclohexyl-3-phenyl-N-(3S)-3-pyrrolidinyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT ***820985-53-3P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of aminopyrrolidines as inhibitors of monoamine uptake)
RN 820985-53-3 HCAPLUS
CN 1-Pyrrolidinecarboxylic acid, 3-[(2-methylpropyl)[(3-phenyl-2-pyridinyl)methyl]amino]-, 1,1-dimethylethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 9 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:780666 HCAPLUS Full-text
DOCUMENT NUMBER: 141:296046
TITLE: Preparation of nitrogen-containing heterocyclic derivatives as chemokine receptor CCR5 antagonists and drugs containing the same as the active ingredient
INVENTOR(S): Nishizawa, Rena; Takaoka, Yoshikazu; Shibayama, Shiro
PATENT ASSIGNEE(S): Ono Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 306 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004080966	A1	20040923	WO 2004-JP3333	20040312
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004220225	A1	20040923	AU 2004-220225	20040312
CA 2517888	AA	20040923	CA 2004-2517888	20040312
EP 1604981	A1	20051214	EP 2004-720257	20040312
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CN 1787996	A	20060614	CN 2004-80013002	20040312
NO 2005004244	A	20051214	NO 2005-4244	20050913
US 2006178399	A1	20060810	US 2005-549120	20050914
PRIORITY APPLN. INFO.:			JP 2003-70347	A 20030314
			JP 2003-385683	A 20031114
			WO 2004-JP3333	A 20040312

OTHER SOURCE(S): MARPAT 141:296046
GI

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AB The title compds. [I; R1 = H, (un)protected acid group; X, Y = a bond, a spacer having 1-3 carbon atoms in the main chain; the ring A or B = (un)substituted 3- to 15-membered allocyclic or heterocyclic ring; the ring D = (un)substituted 3- to 15-membered N-containing heterocyclic ring; R2 = H, cyano, oxo, (un)protected HO, each (un)substituted hydrocarbyl, NH2, or 3- to 15-membered heterocyclyl, :N(OR6); wherein R6 = H, C1-4 alkyl] salts or solvates thereof or prodrugs thereof are prepared These compds. are chemokine receptor CCR5 antagonists and useful in preventing and/or treating human immunodeficiency virus (HIV) infection (in particular, acquired immunodeficiency syndrome), immune diseases (in particular, rejection in organ transplantation), and various inflammatory diseases (in particular, asthma). The various inflammatory diseases may also include nephritis, nephropathy, hepatitis, arthritis, rheumatoid arthritis, rhinitis, conjunctivitis, and ulcerative colitis. The immunol. diseases may further include autoimmune diseases, psoriasis, and multiple sclerosis. They may be also useful for treating and/or preventing allergic diseases (atopic dermatitis, urticaria, allergic bronchopulmonary aspergillosis, or allergic eosinophilic gastroenteritis), ischemic reperfusion injury, acute respiratory distress syndrome, and shock accompanying bacterial infection, diabetes, cancer metastasis. Thus, a solution of 500 mg 1-[4-[4-(methylsulfonylamino)phenoxy]benzyl]piperidine-4- carboxaldehyde, 396 mg N-(tert-butoxycarbonyl)-L-cyclohexylalanine, 0.140 mL n-butylamine, and 0.179 mL 2-morpholinoethyl isocyanide in 13 mL MeOH was stirred at 65° for 12 h, treated with 0.5 mL concentrated HCl, stirred for 2 h, concentrated, treated with 15 mL CH2Cl2 and 15 mL saturated aqueous NaHCO3, and extracted twice with CH2Cl2 to give, after workup, a residue which was heated with 1.25 M AcOH/EtOAc (20 mL) at 70° for 12 h to give, after workup and silica gel chromatog. and salt formation with HCl, N-[4-[4-[[4-[(5S)-1-butyl-5-(cyclohexylmethyl)-3,6-dioxopiperazin-2- yl]piperidin-1-yl]methyl]phenoxy]phenyl]methanesulfonamide hydrochloride. N-butyl-N-[1-[4-[4-(methylsulfonylamino)phenoxy]benzyl]piperidin-4- yl]cyclohexanecarboxamide hydrochloride (II) inhibited the human RANTES-induced temporary increase in cellular Ca2+ ion concentration in CHO stably expressing excess human CCR5 with IC50 of 0.077 μM. Pharmaceutical formulations, e.g. an ampule containing II, were described.

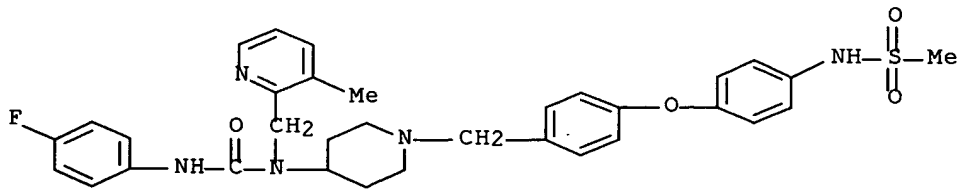
IT ***763931-40-4P 763931-74-4P 763931-75-5P 763931-76-6P 763931-79-9P 763932-05-4P 763932-12-3P 763932-22-5P***

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of nitrogen-containing heterocyclic derivs. as CCR5 antagonists for treating or preventing HIV infection, immune diseases, and inflammatory diseases)

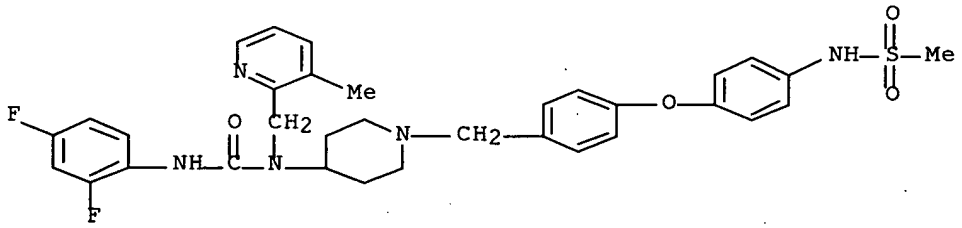
RN 763931-40-4 HCAPLUS

CN Methanesulfonamide, N-[4-[4-[[4-[[[(4-fluorophenyl)amino]carbonyl][(3-methyl-2-pyridinyl)methyl]amino]-1-piperidinyl]methyl]phenoxy]phenyl]-, dihydrochloride (9CI) (CA INDEX NAME)



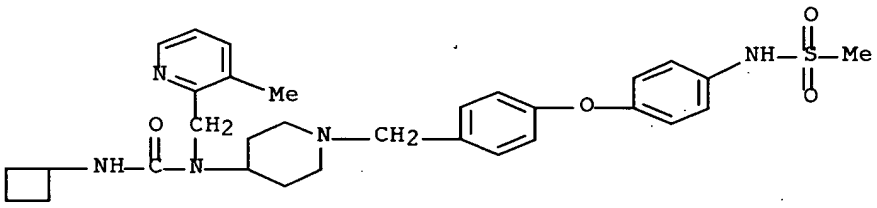
●2 HCl

RN 763931-74-4 HCAPLUS
CN Methanesulfonamide, N-[4-[4-[[4-[[[(2,4-difluorophenyl)amino]carbonyl][(3-methyl-2-pyridinyl)methyl]amino]-1-piperidinyl]methyl]phenoxy]phenyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

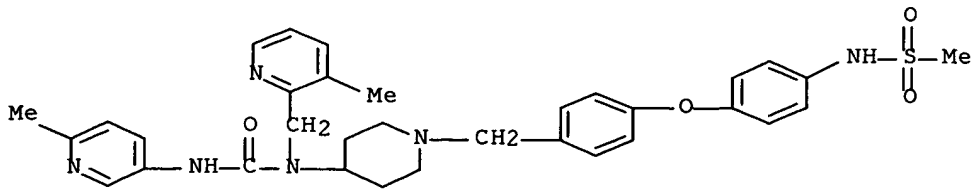
RN 763931-75-5 HCAPLUS
CN Methanesulfonamide, N-[4-[4-[[4-[[(cyclobutylamino)carbonyl][(3-methyl-2-pyridinyl)methyl]amino]-1-piperidinyl]methyl]phenoxy]phenyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 763931-76-6 HCAPLUS

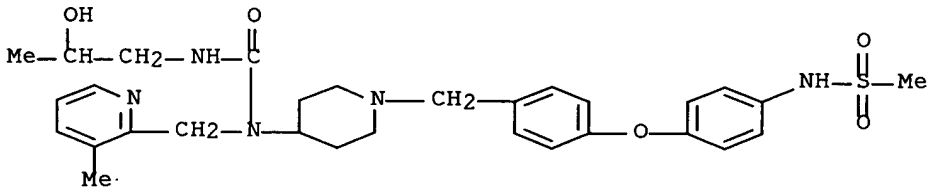
CN Methanesulfonamide, N-[4-[4-[[4-[[[(6-methyl-3-pyridinyl)amino]carbonyl][(3-methyl-2-pyridinyl)methyl]amino]-1-piperidinyl]methyl]phenoxy]phenyl]-, trihydrochloride (9CI) (CA INDEX NAME)



●3 HCl

RN 763931-79-9 HCAPLUS

CN Methanesulfonamide, N-[4-[4-[[4-[[[(2-hydroxypropyl)amino]carbonyl][(3-methyl-2-pyridinyl)methyl]amino]-1-piperidinyl]methyl]phenoxy]phenyl]-, dihydrochloride (9CI) (CA INDEX NAME)

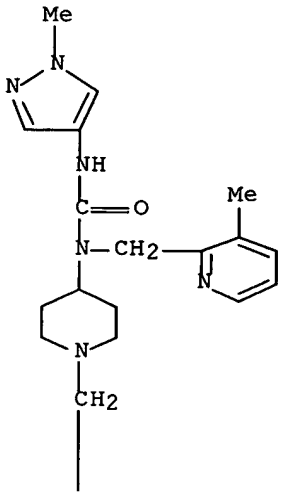


●2 HCl

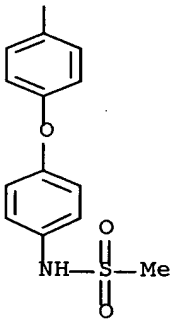
RN 763932-05-4 HCAPLUS

CN Methanesulfonamide, N-[4-[4-[[4-[[[(1-methyl-1H-pyrazol-4-yl)amino]carbonyl][(3-methyl-2-pyridinyl)methyl]amino]-1-piperidinyl]methyl]phenoxy]phenyl]-, trihydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A



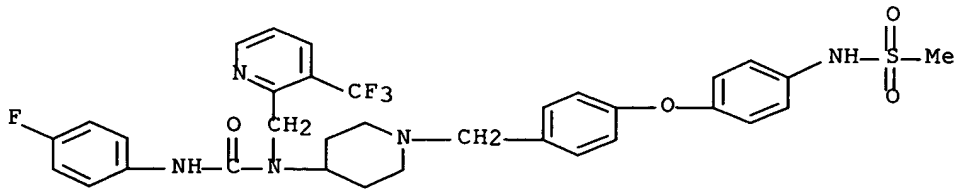
PAGE 2-A



●3 HCl

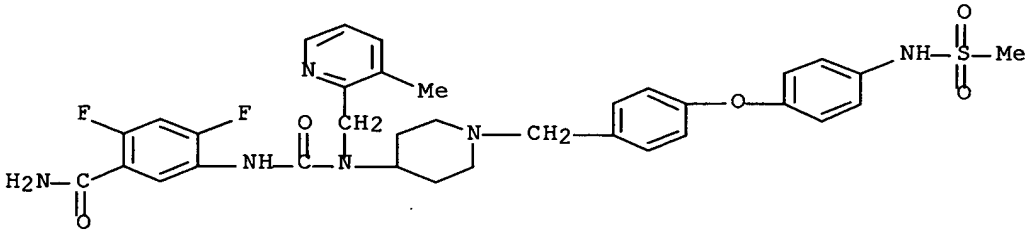
RN 763932-12-3 HCAPLUS

CN Methanesulfonamide, N-[4-[4-[[4-[[[(4-fluorophenyl)amino]carbonyl][[3-(trifluoromethyl)-2-pyridinyl]methyl]amino]-1-piperidinyl]methyl]phenoxy]phenyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 763932-22-5 HCAPLUS
CN Benzamide, 2,4-difluoro-5-[[[[(3-methyl-2-pyridinyl)methyl][1-[[4-[4-[(methylsulfonyl)amino]phenoxy]phenyl]methyl]-4-piperidinyl]amino]carbonyl]amino]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 10 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:732311 HCAPLUS Full-text
DOCUMENT NUMBER: 141:256991
TITLE: Method for labeling phosphorylated peptides, complex compounds used in the methods, process for producing the same, and their intermediates
INVENTOR(S): Koike, Tohru; Kawasaki, Akihiko; Kobashi, Tatsuhiro; Takahagi, Makoto
PATENT ASSIGNEE(S): Kabushiki Kaisha Nard Kenkyusho, Japan
SOURCE: Eur. Pat. Appl., 39 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

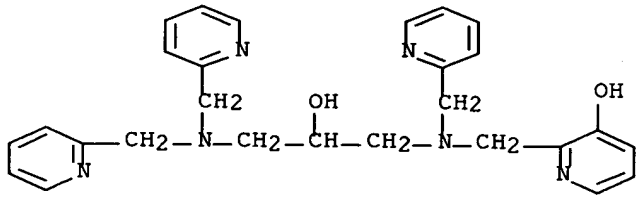
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1455189	A1	20040908	EP 2004-4112	20040224
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				

IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
AU 2004218127 A1 20040916 AU 2004-218127 20040223
CA 2517705 AA 20040916 CA 2004-2517705 20040223
WO 2004078724 A1 20040916 WO 2004-JP2048 20040223
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
US 2004198712 A1 20041007 US 2004-784576 20040223
CN 1526724 A 20040908 CN 2004-10007684 20040224
JP 2006176537 A2 20060706 JP 2006-58217 20060303
PRIORITY APPLN. INFO.: JP 2003-56068 A 20030303
JP 2003-113707 A 20030418
JP 2003-356934 A 20031016
JP 2004-44035 A 20040220
WO 2004-JP2048 A 20040223
JP 2004-94160 A 20040329
JP 2005-514810 A3 20041012
OTHER SOURCE(S): MARPAT 141:256991

AB Provided are a method for easily detecting phosphorylated peptides, namely, proteins, in samples derived from living organisms or the like, a method for selectively adsorbing the phosphorylated peptides, and compds. that are highly coordinated to the phosphorylated peptides and usable in the methods. The complex compound is represented by the formula: wherein X is a linker moiety, and Y is a labeling group. The compound (I) is highly coordinated to a phosphorylated peptide. and has a labeling group. Accordingly, with use of the compound (I), the phosphorylated peptide can be easily identified.

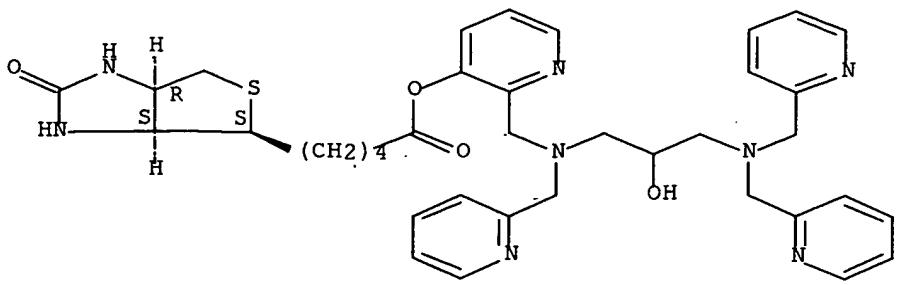
IT ***753451-73-9P 753451-74-0P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(method for labeling phosphorylated peptides, complex compds. used in methods, process for producing same, and their intermediates)

RN 753451-73-9 HCAPLUS
CN 3-Pyridinol, 2-[[[3-[bis(2-pyridinylmethyl)amino]-2-hydroxypropyl](2-pyridinylmethyl)amino]methyl]- (9CI) (CA INDEX NAME)



RN 753451-74-0 HCAPLUS
CN 1H-Thieno[3,4-d]imidazole-4-pentanoic acid, hexahydro-2-oxo-, 2-[[[3-[bis(2-pyridinylmethyl)amino]-2-hydroxypropyl](2-pyridinylmethyl)amino]methyl]-3-pyridinyl ester, (3aS,4S,6aR)- (9CI) (CA INDEX NAME)

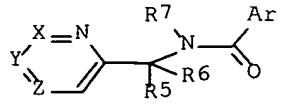
Absolute stereochemistry.



L36 ANSWER 11 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:718519 HCAPLUS Full-text
DOCUMENT NUMBER: 141:225532
TITLE: Preparation of Aryl acid pyrimidinyl/pyridazinyl methyl amides and related compounds as GABAA receptor ligands
INVENTOR(S): Xie, Linghong; Han, Bingsong; Xu, Yuelian
PATENT ASSIGNEE(S): Neurogen Corporation, USA
SOURCE: PCT Int. Appl., 73 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004074259	A1	20040902	WO 2004-IB9	20040216
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2508731	AA	20040902	CA 2004-2508731	20040216
EP 1594848	A1	20051116	EP 2004-711415	20040216
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006517958	T2	20060803	JP 2006-502343	20040216
US 2006135367	A1	20060622	US 2005-544882	20050805
PRIORITY APPLN. INFO.:			US 2003-448271P	P 20030219
			WO 2004-IB9	W 20040216

OTHER SOURCE(S): MARPAT 141:225532
GI



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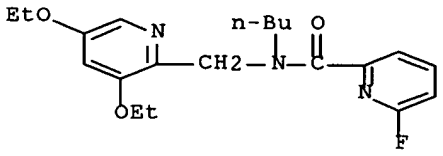
AB Title compds. I [Ar = Ph, naphthyl, etc.; X, Y, Z = N, CR1, such that Y is CR1 if X = N, or Y taken with X or Z to form a 5-membered heterocyclic ring, etc.; R1 = H, halo, NO2, CN, etc.; R4 = OH, NO2, CN, NH2, etc.; R5-6 = H, Me, Et, etc.; R7 = alk(en)yl, cycloalk(en)yl, etc.] are prepared For instance, N-[(4,6-diethoxypyridazin-3-yl)methyl]-2,5-difluoro-N-(3- methylbutyl)benzamide was prepared in 5 steps from 4,6-dichloropyridazine-3- carboxylic acid Et ester. Compds. of the invention had Ki < 1 μM for the GABAA receptor. I are useful for in the treatment of a variety of central nervous system (CNS) disorders in humans, domesticated companion animals, and livestock animals. Compds. provided herein may be administered alone or in combination with one or more other CNS agents to potentiate the effects of the other CNS agent(s).

IT ***748807-66-1P***, 6-Fluoropyridine-2-carboxylic acid N-(butyl)-N-[(3,5-diethoxypyridin-2-yl)methyl]amide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of Aryl acid pyrimidinyl/pyridazinyl Me amides and related compds. as GABAA receptor ligands)

RN 748807-66-1 HCAPLUS

CN 2-Pyridinecarboxamide, N-butyl-N-[(3,5-diethoxy-2-pyridinyl)methyl]-6-fluoro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 12 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:971433 HCAPLUS Full-text

DOCUMENT NUMBER: 140:156145

TITLE: Synthesis and Spectroscopy of μ-Oxo (O2-)-Bridged Heme/Non-heme Diiron Complexes: Models for the Active Site of Nitric Oxide Reductase

AUTHOR(S): Wasser, Ian M.; Martens, Constantinus F.; Verani, Claudio N.; Rentschler, Eva; Huang, Hong-wei; Moeenne-Loccoz, Pierre; Zakharov, Lev N.; Rheingold, Arnold L.; Karlin, Kenneth D.

CORPORATE SOURCE: Department of Chemistry, Johns Hopkins University, Baltimore, MD, 21218, USA

SOURCE: Inorganic Chemistry (2004), 43(2), 651-662

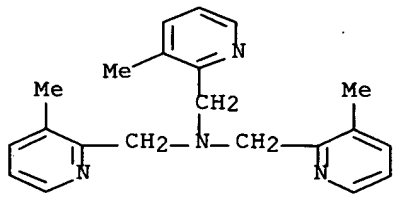
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:156145

AB The authors describe the synthesis and study of heme/nonheme Fe-O-Fe' complexes supported by a porphyrin and the tripodal N ligand TMPA [TMPA = tris(2-pyridylmethyl)amine]. The complete synthesis of [(6L)Fe-O-Fe(X)]+ (1) (X = OMe- or Cl-, 69:31 ratio), where 6L is the dianion of 5-(o-O-[(N,N-bis(2-pyridylmethyl)-2-(6-methoxy)pyridinemethanamino)phenyl])-10,15,20-tris(2,6-difluorophenyl)porphine, is reported. The crystal structure for 1·PF6 reveals an intramol. heme/nonheme diferric complex bridged by an Fe-O-Fe' moiety; ∠(Fe-O-Fe') = 166.7(3)°, and d(Fe···Fe') = 3.556 Å. Crystal data for C70H57ClF12Fe2N8O3P (1·PF6): triclinic, space group P.hivin.1, a 13.185(3), b 14.590(3) Å, c 16.885(4) Å, α 104.219(4), β 91.572(4), γ 107.907(4)°, Z = 2, T = 150(2) K. Complex 1 (X = Cl-) is further characterized by UV-visible, resonance Raman and Mossbauer spectroscopies, MALDI-TOF mass spectrometry and SQUID susceptometry (J = - 114.82 cm-1, S = 0). The authors also synthesized 3-, 4-, and 5-methyl-substituted as well as selectively deuterated TMPA(Fe') complexes and condensed these with the hydroxo complex (F8)FeOH (H2F8 = tetrakis(2,6-difluorophenyl)porphyrin) or (F8-d8)FeOH to yield untethered Fe-O-Fe' analogs. Along with selective deuteration of the methylene hydrogens in TMPA, complete 1H NMR spectroscopic assignments for 1 were accomplished. The magnetic properties of several of the untethered complexes and a comparison to those of 1 are also presented. Complex 1 and related species represent good structural and spectroscopic models for the heme/nonheme diiron active site in the enzyme nitric oxide reductase.

IT ***202192-54-9***, Tris(3-methyl-2-pyridylmethyl)amine
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for preparation of iron tris(pyridylmethyl)amine complex)

RN 202192-54-9 HCAPLUS

CN 2-Pyridinemethanamine, 3-methyl-N,N-bis[(3-methyl-2-pyridinyl)methyl]-(9CI) (CA INDEX NAME)



REFERENCE COUNT: 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

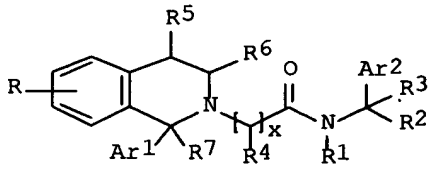
L36 ANSWER 13 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:796667 HCAPLUS Full-text
DOCUMENT NUMBER: 139:307693
TITLE: Preparation of substituted tetrahydroisoquinolines as C5a receptor modulators
INVENTOR(S): Mitchell, Scott; Ohliger, Robert; Zhang, Luyan; Zhao, He; Currie, Kevin; Lee, Kyungae
PATENT ASSIGNEE(S): Neurogen Corporation, USA

SOURCE: PCT Int. Appl., 104 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003082828	A1	20031009	WO 2003-US9046	20030325
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2479930	AA	20031009	CA 2003-2479930	20030325
AU 2003218374	A1	20031013	AU 2003-218374	20030325
EP 1487798	A1	20041222	EP 2003-714371	20030325
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006508894	T2	20060316	JP 2003-580296	20030325
US 2004006069	A1	20040108	US 2003-401135	20030327
US 6777422	B2	20040817		
US 2004204446	A1	20041014	US 2004-824826	20040415
US 6916830	B2	20050712		

PRIORITY APPLN. INFO.:
US 2002-368199P P 20020328
WO 2003-US9046 W 20030325
US 2003-401135 A1 20030327

OTHER SOURCE(S): MARPAT 139:307693
GI



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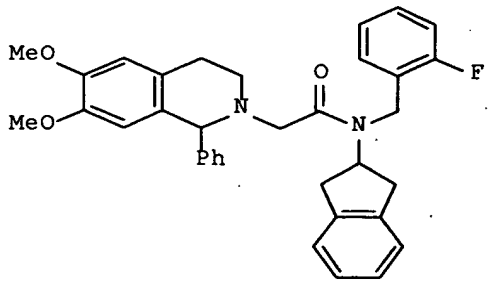


II

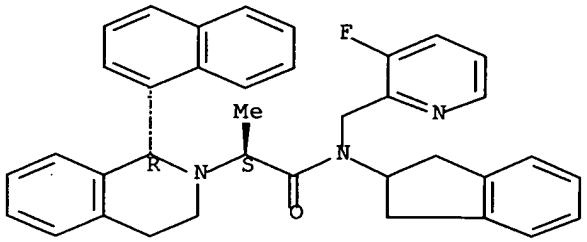
AB The title compds. [I; x = 1-3; R = halo, OH, alkoxy, etc.; R1 = alkyl, alkenyl, cycloalkyl, etc.; R2-R4 = H, halo, alkyl, alkoxy; R5, R6 = H, halo, OH, etc.; R7 = H, alkyl, alkenyl, etc.; Ar1 = (un)substituted Ph, naphthyl, biphenyl, etc.; Ar2 = (un)unsubstituted aryl, heteroaryl] which are ligands that may be used to modulate C5a receptor activity in vivo or in vitro, and are particularly useful in the treatment of conditions associated with pathol. C5a receptor activation in humans, domesticated companion animals and livestock animals, were prepared Thus, reacting 6,7-dimethoxy-1-phenyl-1,2,3,4-tetrahydroisoquinoline.HCl with N-(1-fluorobenzyl)-N-(indan-2-yl)-2-bromoacetamide in the presence of K2CO3 in MeCN afforded II. Preferred compds. I exhibit IC50 values of less than 1 μM in the assay for C5a receptor mediated chemotaxis. Pharmaceutical compns. and methods for using them to treat disorders associated with pathol. C5a receptor activation are provided, as are methods for using such ligands for receptor localization studies.

IT ***610298-28-7P***
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of new aryl imidazoles and related compds. as C5a receptor modulators)

RN 610298-28-7 HCAPLUS

CN 2(1H)-Isoquinolineacetamide, N-(2,3-dihydro-1H-inden-2-yl)-N-[(3-fluoro-2-pyridinyl)methyl]-3,4-dihydro-α-methyl-1-(1-naphthalenyl)-, (αS,1R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

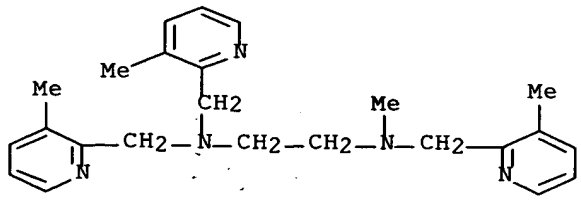
L36 ANSWER 14 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:511444 HCAPLUS Full-text
DOCUMENT NUMBER: 139:87012
TITLE: Support-fixed bleaching catalyst complex compounds suitable as catalysts for peroxide compounds
INVENTOR(S): Gentschev, Pavel; Doering, Steve; Breyer, Jacques; Machin, Antonio
PATENT ASSIGNEE(S): Henkel Kommanditgesellschaft Auf Aktien, Germany
SOURCE: PCT Int. Appl., 133 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003054128	A1	20030703	WO 2002-EP14290	20021216
W: AU, BR, BY, CA, CN, DZ, HU, ID, IL, IN, JP, KR, MX, NO, NZ, PL, RO, RU, SG, UA, US, UZ, VN, YU, ZA				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR				
DE 10163331	A1	20030710	DE 2001-10163331	20011221
AU 2002360982	A1	20030709	AU 2002-360982	20021216
EP 1456337	A1	20040915	EP 2002-795195	20021216
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, SK				
US 2004266641	A1	20041230	US 2004-873071	20040621
PRIORITY APPLN. INFO.:			DE 2001-10163331 A	20011221
			WO 2002-EP14290 W	20021216

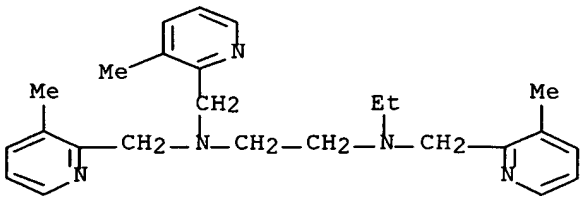
AB The invention relates to support-fixed bleaching catalyst(s) suitable for the catalysis of peroxide compds., characterized in that the support-fixed bleaching catalyst(s) is/are covalently bonded to a support by means of at least one organic ligand of the bleaching catalyst. The bleaching catalyst(s) form(s) a complex with at least one transition metal. The invention further relates to support-fixed bleaching catalysts for the catalysis of peroxide compds., where at least one ligand, covalently bonded to a support, is a transition-metal-free ligand, which chelates with a transition metal, derived from another source, preferably from the bleaching composition and/or added water and thus forms the complex with a transition metal. These bleaching catalysts are useful in laundering of colored fabrics at low temps. A typical catalyst was manufactured by reaction of chloromethylated polystyrene with bis(2-pyridylmethyl)amine, and complexing the products with Fe(ClO4)3.

IT ***260395-26-4DP***, N-Methyl-N,N',N'-tris(3-methyl-2-pyridylmethyl)ethylenediamine, reaction products with polymers, transition metal complexes ***260395-27-5DP***, N,N',N'-Tris(3-methyl-2-pyridylmethyl)-N-ethylethylenediamine, reaction products with polymers, transition metal complexes
RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)
(polymer-supported transition metal complexes as catalysts for peroxide bleaching agents)

RN 260395-26-4 HCAPLUS
CN 1,2-Ethanediamine, N-methyl-N,N',N'-tris[(3-methyl-2-pyridinyl)methyl]- (9CI) (CA INDEX NAME)



RN 260395-27-5 HCAPLUS
CN 1,2-Ethanediamine, N-ethyl-N,N',N'-tris[(3-methyl-2-pyridinyl)methyl]- (9CI) (CA INDEX NAME)

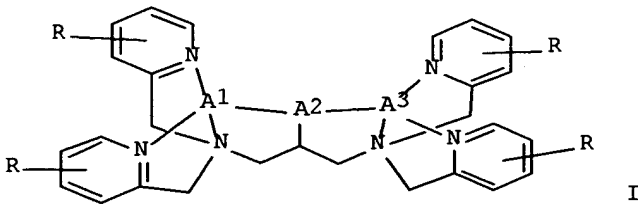


REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 15 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:511300 HCAPLUS Full-text
DOCUMENT NUMBER: 139:94262
TITLE: Preparation of zinc complexes capable of scavenging substances bearing anionic substituents
INVENTOR(S): Koike, Tohru; Suzuki, Masatatsu; Shionoya, Mitsuhiko
PATENT ASSIGNEE(S): Japan
SOURCE: PCT Int. Appl., 61 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003053932	A1	20030703	WO 2002-JP13341	20021220
W: DE, JP, US				
US 2005038258	A1	20050217	US 2004-878131	20040621
PRIORITY APPLN. INFO.:			JP 2001-390395 A	20011221
			WO 2002-JP13341 A1	20021220

OTHER SOURCE(S): MARPAT 139:94262
GI



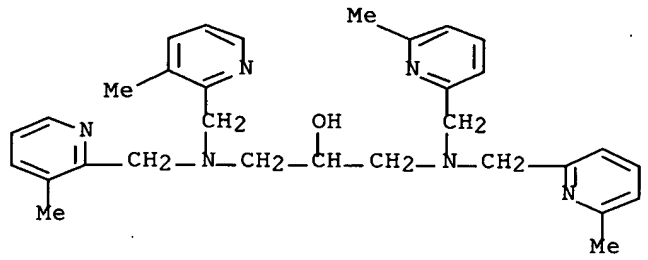
I

AB The title compds. I [R = H, C1-C16 alkyl, etc.; A1 = A3 = Zn2+; A2 = O-] are prepared I are useful as additives in mass spectrometry, NMR, etc.
IT ***553645-33-3***
RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of zinc complexes capable of scavenging substances bearing anionic substituents useful in mass spectrometry and NMR)

RN 553645-33-3 HCAPLUS

CN 2-Propanol, 1-[bis[(3-methyl-2-pyridinyl)methyl]amino]-3-[bis[(6-methyl-2-pyridinyl)methyl]amino]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 16 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:813938 HCAPLUS Full-text

DOCUMENT NUMBER: 137:337907

TITLE: Preparation of N-(heteroarylalkyl)acylamides as CXCR3 antagonists for treatment of inflammatory or immune conditions

INVENTOR(S): Medina, Julio C.; Johnson, Michael G.; Li, An-Rong; Liu, Jiwen; Huang, Alan Xi; Zhu, Liusheng; Marcus, Andrew P.

PATENT ASSIGNEE(S): Tularik Inc., USA

SOURCE: PCT Int. Appl., 205 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

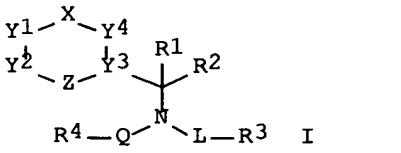
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002083143	A1	20021024	WO 2001-US47850	20011211
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2431553	AA	20021024	CA 2001-2431553	20011211
US 2002169159	A1	20021114	US 2001-15532	20011211
US 6964967	B2	20051115		
EP 1343505	A1	20030917	EP 2001-273533	20011211
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				

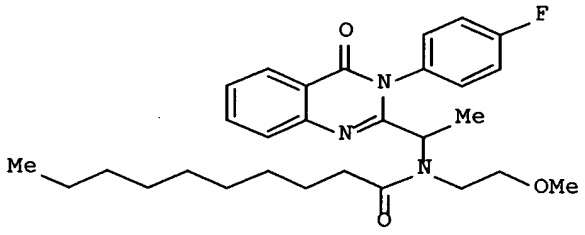
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004536796	T2	20041209	JP 2002-580947	20011211
CN 1575177	A	20050202	CN 2001-822596	20011211
BR 2001016096	A	20051018	BR 2001-16096	20011211
NZ 526622	A	20060728	NZ 2001-526622	20011211
US 2003069234	A1	20030410	US 2002-164690	20020606
US 6794379	B2	20040921		
US 2003055054	A1	20030320	US 2002-231895	20020829
US 7053215	B2	20060530		
ZA 2003004342	A	20050509	ZA 2003-4342	20030603
NO 2003002612	A	20030805	NO 2003-2612	20030610
US 2005075333	A1	20050407	US 2004-946935	20040921
US 7067662	B2	20060627		
US 2006116388	A1	20060601	US 2006-332054	20060113
PRIORITY APPLN. INFO.:			US 2000-255241P	P 20001211
			US 2001-296499P	P 20010606
			US 2001-15532	A1 20011211
			WO 2001-US47850	W 20011211
			US 2002-164690	A1 20020606
			US 2002-231895	A1 20020829

OTHER SOURCE(S): MARPAT 137:337907

GI



I



II

AB Title compds. I [wherein X = a bond, CO, CR5R6, CR5:, SO, SO2, or N: ; Z = a bond, N:, O, S, NR17, or CR7: ; with the proviso that X and Z are not both a bond; L = CO-alkylene or (hetero)alkylene; Q = (hetero)alkylene, CO, OCO, NR8CO, CH2CO, CH2SO, or CH2SO2; or NLQ = heterocyclyl; R1 and R2 = independently H, (hetero)alkyl, or (hetero)aryl; or CR1R2 = (hetero)cyclyl; or CNR2L = heterocyclyl; R3 = OH, alkoxy, NH2, (di)alkylamino, heteroalkyl, heterocyclyl, acylaminoamidino, guanidino, ureido, CN, heteroaryl, carbamoyl, or carboxy; R4 = (hetero)alkyl, (hetero)aryl, etc.; R5 and R6 = independently H, (hetero)alkyl, or (hetero)aryl; or CR5R6 = a ring; R7 and R8 = independently H, (hetero)alkyl, or (hetero)aryl; Y1 and Y2 = independently CR12: N:, O, S, or NR13; Y3 = N or C, wherein C shares a double bond with either Z or Y4; Y4 = NR14, CR14:, N:, NR14CR15R16; R12 = H, halo, OH, NH2, (di)alkylamino, (hetero)alkyl, or (hetero)aryl, with provisos; R13 = H,

(hetero)alkyl, (hetero)aryl, etc.; R14 = (hetero)alkyl, (hetero)aryl, etc.; R15 and R16 = independently H or (hetero)alkyl; R17 = H, (hetero)alkyl, (hetero)aryl, etc.; with provisos] were prepared as chemokine receptor modulators, in particular CXCR3 antagonists. For example, anthranilic acid was acylated with propionyl chloride and the amide cyclized using acetic anhydride to give 2-ethylbenzo[d][1,3]oxazine-4-one. Treatment with 4-fluoroaniline, followed by ethylene glycol and NaOH afforded 2-ethyl-3-(4-fluorophenyl)- 3H-quinazolin-4-one. Bromination and stepwise addition of 1-amino-2-methoxyethane and decanoyl chloride produced the decanoic acid (quinazolinylethyl)(methoxyethyl)amide II. Approx. one third of the 101 invention compds. tested in a CXCR3 binding assay displayed activity with IC50 values of < 1 μM. I are useful for the treatment of inflammatory and immunoregulatory disorders and diseases, such as multiple sclerosis, rheumatoid arthritis, and type I diabetes (no data).

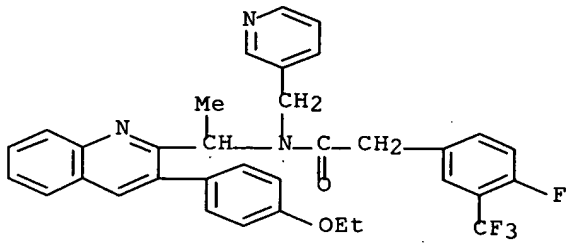
IT ***473720-00-2P***

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(CXCR3 antagonist; preparation of N-(heteroarylalkyl)acylamides as CXCR3 antagonists for treatment of inflammatory or immune conditions)

RN 473720-00-2 HCAPLUS

CN Benzeneacetamide, N-[1-[3-(4-ethoxyphenyl)-2-quinolinyl]ethyl]-4-fluoro-N-(3-pyridinylmethyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 17 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:813424 HCAPLUS Full-text

DOCUMENT NUMBER: 138:153131

TITLE: New manganese catalysts for alcohol oxidation

AUTHOR(S): Brinksma, Jelle; Rispens, Minze T.; Hage, Ronald; Feringa, Ben L.

CORPORATE SOURCE: Laboratory of Organic Chemistry, Stratingh Institute, University of Groningen, Groningen, 9747 AG, Neth.

SOURCE: Inorganica Chimica Acta (2002), 337, 75-82
CODEN: ICHAA3; ISSN: 0020-1693

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:153131

AB The in situ prepared manganese complexes based on ligand N,N,N',N'-tetrakis(2-pyridylmethyl)-1,3-propanediamine have been used in the catalytic oxidation of alcs. to aldehydes or ketones. Highly active and selective catalysts were

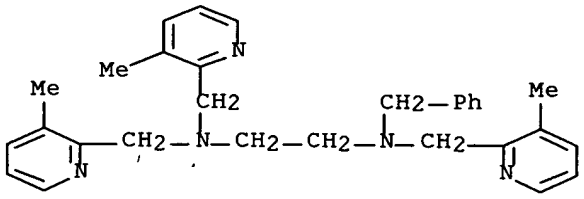
found with excellent turnover nos. (up to 900) using aqueous hydrogen peroxide as oxidant at ambient temps. EPR spectroscopy and electrospray mass spectrometry has indicated that dinuclear species may be involved in the catalytic oxidns. Comparing the rate of oxidation of benzyl-d7 alc. with that of benzyl alc. by the different catalysts yielded isotope effects (kH/kD) of 2.2-4.3. Although the exact nature of the oxidizing species has not been elucidated, these results indicate that hydroxyl radicals are not involved in these processes.

IT ***260395-28-6 494825-18-2***

RL: CAT (Catalyst use); USES (Uses)
(catalytically active ligand; in situ prepared Mn complexes based on ligand N,N,N',N'-tetrakis(2-pyridylmethyl)-1,3-propanediamine as selective oxidation catalysts for primary and secondary alcs. using aqueous hydrogen peroxide as oxidant)

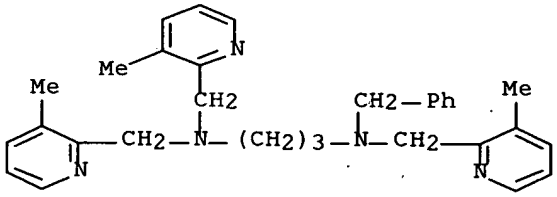
RN 260395-28-6 HCAPLUS

CN 1,2-Ethanediamine, N,N,N'-tris[(3-methyl-2-pyridinyl)methyl]-N'-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 494825-18-2 HCAPLUS

CN 1,3-Propanediamine, N,N,N'-tris[(3-methyl-2-pyridinyl)methyl]-N'-(phenylmethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 18 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:893482 HCAPLUS Full-text

DOCUMENT NUMBER: 136:193225

TITLE: Coordination of semiquinone and superoxide radical anions to the zinc ion in SOD model complexes that act as the key step in disproportionation of the radical anions

AUTHOR(S): Ohtsu, Hideki; Fukuzumi, Shunichi

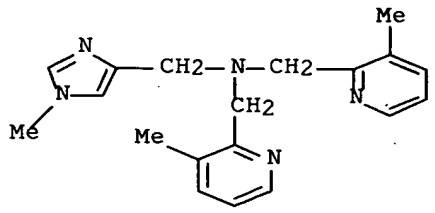
CORPORATE SOURCE: Department of Material and Life Science Graduate School of Engineering, Osaka University CREST, JAPAN Science and Technology Corporation, Suita, 565-0871, Japan
SOURCE: Chemistry--A European Journal (2001), 7(22), 4947-4953
CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:193225

AB Reactions of imidazolate-bridged CuII-ZnII heterodinuclear and CuII-CuII homodinuclear complexes, [CuIIZnII(bdpi)(CH3CN)2](ClO4)3·2CH3CN (1) and [CuII2(bdpi)(CH3CN)2](ClO4)3·CH3CN·3H2O (2) (Hbdpi = 4,5-bis(di(2-pyridylmethyl)aminomethyl)imidazole), with the p-benzosemiquinone radical anion (Q•-) have been examined to provide mechanistic insight into the role of the ZnII ion in copper-zinc superoxide dismutase (Cu,Zn-SOD). The addition of less than one equivalent of Q•- to a deaerated solution of 1 or 2 in propionitrile at -80° results in the oxidation of Q•- accompanied by the appearance of a new absorption band at 585 nm due to the CuI-Q complex (3 or 4, resp.), the absorbance of which increases linearly with the increase in Q•- concentration Both the resonance Raman spectra of 3 and 4 exhibit a strong resonance-enhanced Raman band at 1580 cm-1, which can be assigned to a CO stretching vibration in the CuI-Q complexes. Further addition of Q•- to a deaerated solution of 3 in propionitrile results in the reduction of Q•-, whereas no reduction of Q•- occurs with 4, which does not contain the ZnII ion. Thus, the coordination of Q•- to the ZnII ion is essential for the reduction of Q•- by the CuI ion in 3. The coordination of O2•- and Q•- to the ZnII ion has been confirmed by the electronic and ESR spectra of the O2•- and Q•- complexes with mononuclear ZnII complexes, [ZnII{MeIm(Py)2}(CH3CN)](ClO4)2 (5) and [ZnII{MeIm(Me)2}(H2O)](ClO4)2 (6) (MeIm(Py)2 = (1-methyl-4-imidazolylmethyl)bis(2-pyridylmethyl)amine, MeIm(Me)2 = (1-methyl-4-imidazolylmethyl)bis(6-methyl-2-pyridylmethyl)amine). The binding energies of O2•- with the ZnII ion in 5 and 6 have been evaluated from the deviation of the g values of the ESR spectra from the free spin value.

IT ***399024-69-2P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and complexation with zinc)

RN 399024-69-2 HCAPLUS

CN 2-Pyridinemethanamine, 3-methyl-N-[(1-methyl-1H-imidazol-4-yl)methyl]-N-[(3-methyl-2-pyridinyl)methyl]- (9CI) (CA INDEX NAME)



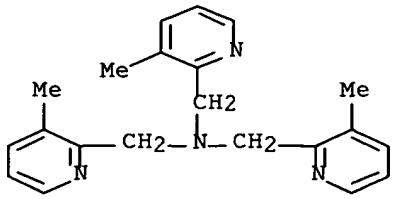
REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 19 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:417457 HCAPLUS Full-text
DOCUMENT NUMBER: 135:164014
TITLE: Stereospecific Alkane Hydroxylation by Non-Heme Iron Catalysts: Mechanistic Evidence for an FeV:O Active Species
AUTHOR(S): Chen, Kui; Que, Lawrence, Jr.
CORPORATE SOURCE: Department of Chemistry and Center for Metals in Biocatalysis, University of Minnesota, Minneapolis, MN, 55455, USA
SOURCE: Journal of the American Chemical Society (2001), 123(26), 6327-6337
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:164014

AB High-valent iron-oxo species have frequently been invoked in the oxidation of hydrocarbons by both heme and non-heme enzymes. Although a formally FeV:O species, i.e., [(Por•)FeIV:O]+, has been widely accepted as the key oxidant in stereospecific alkane hydroxylation by heme systems, it is not established that such a high-valent state can be accessed by a non-heme ligand environment. Herein we report a systematic study on alkane oxidns. with H2O2 catalyzed by a group of non-heme iron complexes, i.e., [FeII(TPA)(CH3CN)2]2+ (1, TPA = tris(2-pyridylmethyl)amine) and its α- and β-substituted analogs. The reactivity patterns of this family of FeII(TPA) catalysts can be modulated by the electronic and steric properties of the ligand environment, which affects the spin states of a common FeIII-OOH intermediate. Such an FeIII-peroxo species is high-spin when the TPA ligand has two or three α-substituents and is proposed to be directly responsible for the selective C-H bond cleavage of the alkane substrate. The thus-generated alkyl radicals, however, have relatively long lifetimes and are susceptible to radical epimerization and trapping by O2. On the other hand, 1 and the β-substituted FeII(TPA) complexes catalyze stereospecific alkane hydroxylation by a mechanism involving both a low-spin FeIII-OOH intermediate and an FeV:O species derived from O-O bond heterolysis. We propose that the heterolysis pathway is promoted by two factors: (a) the low-spin iron(III) center which weakens the O-O bond and (b) the binding of an adjacent water ligand that can hydrogen bond to the terminal oxygen of the hydroperoxo group and facilitate the departure of the hydroxide. Evidence for the FeV:O species comes from isotope-labeling studies showing incorporation of 18O from H218O into the alc. products. 18O-incorporation occurs by H218O binding to the low-spin FeIII-OOH intermediate, its conversion to a cis-H18O-FeV:O species, and then oxo-hydroxo tautomerization. The relative contributions of the two pathways of this dual-oxidant mechanism are affected by both the electron donating ability of the TPA ligand and the strength of the C-H bond to be broken. These studies thus serve as a synthetic precedent for an FeV:O species in the oxygen activation mechanisms postulated for non-heme iron enzymes such as methane monooxygenase and Rieske dioxygenases.

IT ***202192-54-9***
RL: RCT (Reactant); RACT (Reactant or reagent)
(stereospecific alkane hydroxylation by non-heme iron catalysts and mechanistic evidence for FeV:O active species)

RN 202192-54-9 HCAPLUS
CN 2-Pyridinemethanamine, 3-methyl-N,N-bis[(3-methyl-2-pyridinyl)methyl]- (9CI) (CA INDEX NAME)



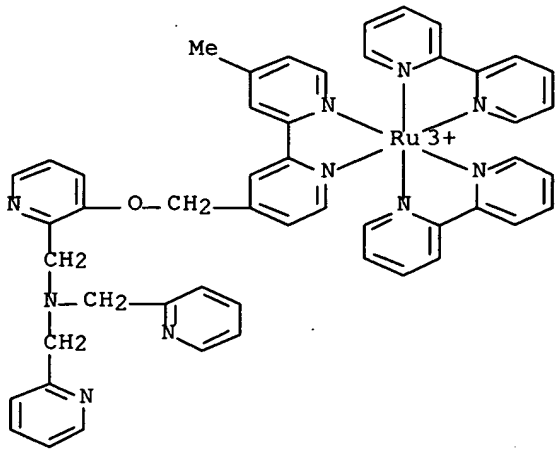
REFERENCE COUNT: 85 THERE ARE 85 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 20 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:257215 HCAPLUS Full-text
DOCUMENT NUMBER: 135:40010
TITLE: Covalently linked ruthenium(II)-manganese(II) complexes: distance dependence of quenching and electron transfer
AUTHOR(S): Berg, Katja E.; Tran, Anh; Raymond, Mary Katherine; Abrahamsson, Malin; Wolny, Juliusz; Redon, Sophie; Andersson, Mikael; Sun, Licheng; Styring, Stenbjorn; Hammarstrom, Leif; Toftlund, Hans; Akermark, Bjorn
CORPORATE SOURCE: Dept. of Organic Chemistry, Stockholm University, Stockholm, 106 91, Swed.
SOURCE: European Journal of Inorganic Chemistry (2001), (4), 1019-1029
CODEN: EJICFO; ISSN: 1434-1948
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:40010

AB Continuing the authors' development of artificial models for photosystem II in green plants, compds. were prepared in which a Ru(bpy)32+ photosensitizer is covalently linked to a Mn(II) electron donor. In addition to a trispicolylamine ligand, two other Mn ligands, dipicolylamine and aminodiacetic acid, were introduced to study ligands that are appropriate for the construction of Mn dimers with open coordination sites for the binding of H2O. Coordination equilibrium of the Mn ions were monitored by EPR. The interactions between the Ru and Mn moieties were probed by flash photolysis, cyclic voltammetry and steady-state and time-resolved emission measurements. The quenching of the RuII excited state by MnII is rapid in complexes with short Ru-Mn distances. Nevertheless, each RuII species could be photooxidized by bimol. quenching with methylviologen, and the subsequent electron transfer from MnII to RuIII could be monitored.

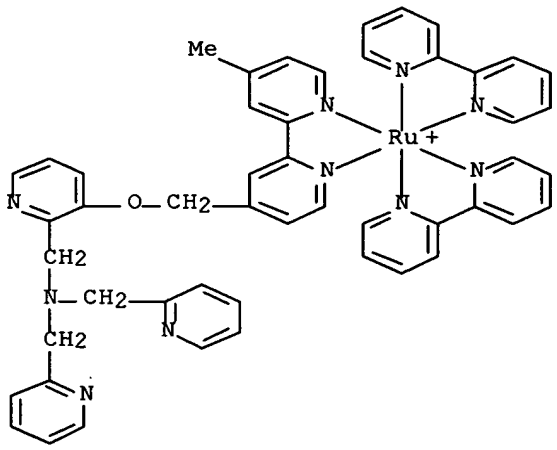
IT ***344367-78-8 344367-79-9***
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(elec. potential of couple containing)

RN 344367-78-8 HCAPLUS
CN Ruthenium(3+), bis(2,2'-bipyridine-κN1,κN1')[3-[(4'-methyl[2,2'-bipyridin]-4-yl-κN1,κN1')methoxy]-N,N-bis(2-pyridinylmethyl)-2-pyridinemethanamine]-, (OC-6-33)- (9CI) (CA INDEX NAME)



RN 344367-79-9 HCAPLUS

CN Ruthenium(1+), bis(2,2'-bipyridine-κN1,κN1')[3-[(4'-methyl[2,2'-bipyridin]-4-yl-κN1,κN1')methoxy]-N,N-bis(2-pyridinylmethyl)-2-pyridinemethanamine]-, (OC-6-33)- (9CI) (CA INDEX NAME)



IT ***344367-63-1P***

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

(preparation and complexation with manganese dichloride and cyclic voltammetry and photophys.)

RN 344367-63-1 HCAPLUS

CN Ruthenium(2+), bis(2,2'-bipyridine-κN1,κN1')[3-[(4'-

methyl[2,2'-bipyridin]-4-yl-κN1,κN1')methoxy]-N,N-bis(2-pyridinylmethyl)-2-pyridinemethanamine]-, (OC-6-33)-, bis[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

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CRN 344367-62-0
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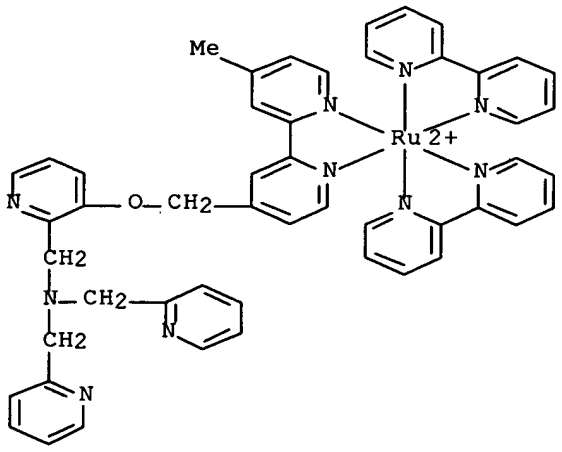
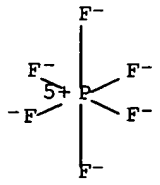
CCI CCS

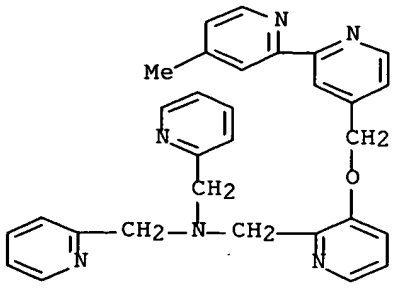


CM 2

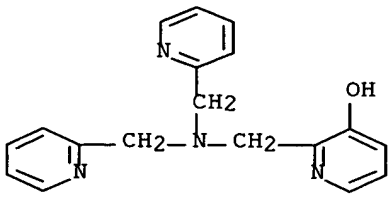
CRN 16919-18-9
CMF F6 P
CCI CCS



IT ***344367-68-6DP***, manganese ruthenium bipyridine complex
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(preparation and cyclic voltammetry and photophys.)
RN 344367-68-6 HCAPLUS
CN 2-Pyridinemethanamine, 3-[(4'-methyl[2,2'-bipyridin]-4-yl)methoxy]-N,N-bis(2-pyridinylmethyl)- (9CI) (CA INDEX NAME)



IT ***344367-61-9P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactant for preparation of manganese ruthenium complexes with
bipyridine having dipicolylamine or aminodiacetic acid pendants)
RN 344367-61-9 HCAPLUS
CN 3-Pyridinol, 2-[[bis(2-pyridinylmethyl)amino]methyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

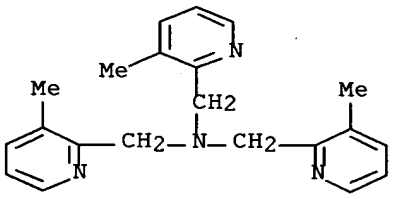
L36 ANSWER 21 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:247836 HCAPLUS Full-text
DOCUMENT NUMBER: 135:39981
TITLE: Fine Tuning of the Interaction between the Copper(I) and Disulfide Bond. Formation of a Bis(μ-thiolato)dicopper(II) Complex by Reductive Cleavage of the Disulfide Bond with Copper(I)
AUTHOR(S): Itoh, Shinobu; Nagagawa, Motonobu; Fukuzumi, Shunichi
CORPORATE SOURCE: Department of Chemistry Graduate School of Science, Osaka City University, Sumiyoshi-ku Osaka, 558-8585, Japan
SOURCE: Journal of the American Chemical Society (2001), 123(17), 4087-4088
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 22 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:216947 HCAPLUS Full-text
DOCUMENT NUMBER: 135:86033
TITLE: Chiral induction upon coordination to form an enantiomeric bis-chelate ruthenium(II)-tris(3-methyl-2-pyridylmethyl)amine complex
AUTHOR(S): Kojima, Takahiko; Matsuda, Yoshihisa
CORPORATE SOURCE: Graduate School of Sciences, Department of Chemistry, Kyushu University, Higashi-Ku, Hakozaki, Fukuoka, 812-8581, Japan
SOURCE: Journal of the Chemical Society, Dalton Transactions (2001), (7), 958-960
CODEN: JCSDAA; ISSN: 1472-7773
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:86033

AB The reaction of tris(3-methyl-2-pyridylmethyl)amine with RuCl3 in MeOH in the presence of NEt3 under N2 gave a novel bis-chelate Ru(II) mononuclear complex [Ru(3-Me3-TPA)2](PF6)2. (1). The crystal structure of 1 was revealed to be C2-sym. and chiral due to the asym. tertiary N's and a unit cell contains two (R,R) and two (S,S) isomers to form a racemic crystal. The isolated isomer turned out to be a cis isomer. Chiral induction to a C3-sym. and nonprochiral tris(3-methyl-2-pyridylmethyl)amine was achieved upon coordination to a Ru(II) center by forming a stable fac-cis bis-chelate complex selectively and 1H NMR spectroscopy showed that the chirality is maintained even in solution

IT ***202192-54-9***, Tris(3-methyl-2-pyridylmethyl)amine
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of enantiomeric bis-chelate ruthenium(II) tris(3-methyl-2-pyridylmethyl)amine complex)
RN 202192-54-9 HCAPLUS
CN 2-Pyridinemethanamine, 3-methyl-N,N-bis[(3-methyl-2-pyridinyl)methyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 23 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:168088 HCAPLUS Full-text
DOCUMENT NUMBER: 134:224341
TITLE: Bleaching composition and method for bleaching a substrate such as laundered fabrics with atmospheric oxygen or air

LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:39981

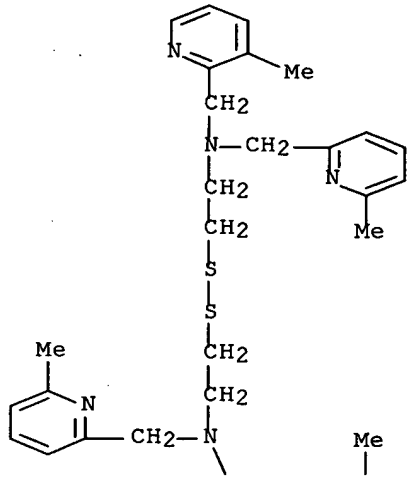
AB [Cu(MeCN)4]ClO4 reacted with bis-2-(bis(2-(2-pyridyl)ethyl)amino)ethyl disulfide (L) or bis(2-bis(2-bis((6-methyl-2-pyridyl)methyl)amino)ethyl) disulfide (L1) gave [Cu2L](ClO4)2 (I) and [Cu2L1](ClO4)2 (II) whereas the reaction with bis-2(bis(2-pyridylmethyl)amino)ethyl disulfide (L2) gave [Cu2L32](ClO4)2 (III) (H2L3 = 2-(bis(2-pyridylmethyl)amino)ethylthiol) as a result of disulfide bond cleavage. I, II and III were characterized by single crystal structural anal. and cyclic voltammetry. I.MeCN is triclinic, space group P1, Z = 2, R = 0.129, Rw = 0.221. II is monoclinic, space group P2/n, Z = 2, R = 0.228, Rw = 0.189. III.MeCN is orthorhombic, space group Pna21, Z = 4, R = 0.075, Rw = 0.120. In I the Cu(I) atoms are tetrahedral whereas in II the Cu(I) atoms are distorted trigonal pyramidal. In III the Cu(II) atoms are square pyramidal. The preparation of L, L1 and L2 is described.

IT ***343627-74-7P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and complexation with copper(I))

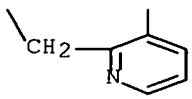
RN 343627-74-7 HCAPLUS

CN 2-Pyridinemethanamine, N,N'-(dithiodi-2,1-ethanediyl)bis[3-methyl-N-[(6-methyl-2-pyridinyl)methyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS

INVENTOR(S): Carina, Riccardo Filippo; Fox, Stephen Paul; Kalmeijer, Robertus Everardus; Karlin, Kenneth Daniel; Thijssen, Rob; Twisker, Robin Stefan
PATENT ASSIGNEE(S): Unilever PLC, UK; Unilever NV; Hindustan Lever Limited
SOURCE: PCT Int. Appl., 49 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 13
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001016261	A2	20010308	WO 2000-EP8078	20000816
WO 2001016261	A3	20010830		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW				
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WO 2000012667	A1	20000309	WO 1999-GB2876	19990901
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WO 2000012808	A1	20000309	WO 1999-GB2878	19990901
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CA 2383935	AA	20010308	CA 2000-2383935	20000816
EP 1208185	A2	20020529	EP 2000-953179	20000816
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BR 2000013737	A	20020604	BR 2000-13737	20000816
PRIORITY APPLN. INFO.:			WO 1999-GB2876 W	19990901
			WO 1999-GB2878 W	19990901
			GB 2000-6961 A	20000322
			GB 1998-19046 A	19980901
			GB 1999-6474 A	19990319
			GB 1999-7713 A	19990401
			GB 1999-7714 A	19990401
			WO 2000-EP8078 W	20000816

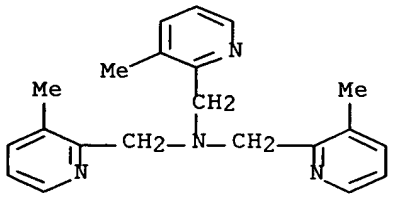
OTHER SOURCE(S): MARPAT 134:224341

AB Bleaching a substrate comprises applying to the substrate, in an aqueous medium, a specified ligand which forms a complex with a transition metal, for

bleaching of the substrate by atmospheric O. An aqueous bleaching composition is substantially devoid of peroxygen bleach or a peroxy-based or peroxy-generating bleach system. The catalyst may be used in dry form, or in a liquor that is then dried, such as an aqueous spray-on fabric treatment fluid or a wash liquor for laundry cleaning, or a nonaq. dry cleaning fluid or spray-on aerosol fluid. A typical complex of tris(3-methylpyridin-2-yl methyl)amine ligand complex with Fe(ClO4)2.6H2O showed good performance (curry oil stained fabric δE 17) in alkaline wash.

IT ***202192-54-9D***, iron and manganese complexes
RL: CAT (Catalyst use); USES (Uses)
(composition for bleaching a laundered fabrics with atmospheric oxygen or air)

RN 202192-54-9 HCAPLUS
CN 2-Pyridinemethanamine, 3-methyl-N,N-bis[(3-methyl-2-pyridinyl)methyl]- (9CI) (CA INDEX NAME)



RL: IMF (Industrial manufacture); PREP (Preparation)
(ligand; compn. for bleaching a laundered fabrics with atm. oxygen or air

L36 ANSWER 24 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:725738 HCAPLUS Full-text
DOCUMENT NUMBER: 133:311157
TITLE: Composition containing transition metal complex for catalytically bleaching laundry fabrics with atmospheric oxygen
INVENTOR(S): Appel, Adrianus Cornelis Maria; Delroisse, Michel Gilbert Jose; Hage, Ronald; Tetard, David; Twisker, Robin Stefan
PATENT ASSIGNEE(S): Unilever PLC, UK; Unilever N. V.; Hindustan Lever Limited
SOURCE: PCT Int. Appl., 70 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 13
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000060043	A1	20001012	WO 2000-EP2587	20000322

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,

SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

WO 2000012667 A1 20000309 WO 1999-GB2876 19990901
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WO 2000012808 A1 20000309 WO 1999-GB2878 19990901
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EP 1433840 A1 20040630 EP 2004-7615 19990901
R: BE, DE, ES, FR, GB, IT

ZA 2001006939 A 20020822 ZA 2001-6939 20010822

PRIORITY APPLN. INFO.:

GB 1999-7713	A	19990401
GB 1999-7714	A	19990401
WO 1999-GB2876	W	19990901
WO 1999-GB2878	W	19990901
GB 2000-4858	A	20000229
GB 1998-19046	A	19980901
GB 1999-6474	A	19990319
EP 1999-943083	A3	19990901

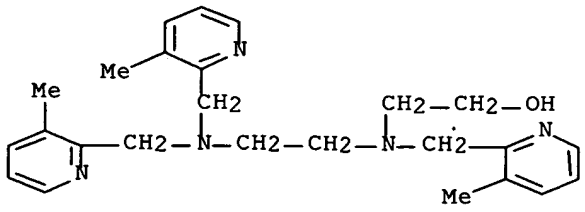
OTHER SOURCE(S): MARPAT 133:311157

AB The title method comprises applying to the substrate, in an aqueous bleaching composition containing a ligand complex with a transition metal, the complex catalyzing bleaching of the substrate by atmospheric O. Also the aqueous bleaching composition is substantially devoid of peroxygen bleach or a peroxy-based or -generating bleach system. Tomato stained cloths were bleached in the presence of a cleaner containing surfactant and 10 μM [Fe(N-methyl-N,N',N'- tris(3-methylpyridin-2-ylmethyl)ethylenediamine)Cl](PF6)(preparation given), showing a color difference (pH 8) 17; vs. 3 for a blank and 2 using peroxide source bleach.

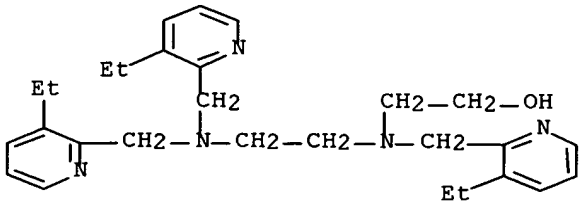
IT ***260395-29-7 302543-44-8***
RL: CAT (Catalyst use); USES (Uses)
(ligand; composition containing transition metal complex for catalytically bleaching laundry fabrics with atmospheric oxygen)

RN 260395-29-7 HCAPLUS

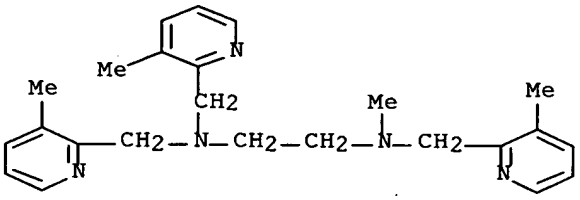
CN Ethanol, 2-[[2-[bis[(3-methyl-2-pyridinyl)methyl]amino]ethyl][(3-methyl-2-pyridinyl)methyl]amino]- (9CI) (CA INDEX NAME)



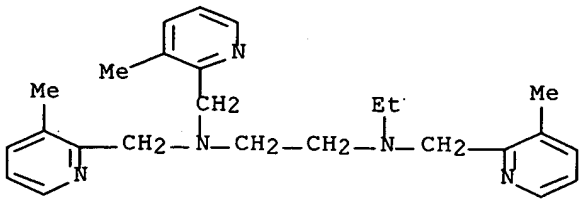
RN 302543-44-8 HCAPLUS
CN Ethanol, 2-[[2-[bis[(3-ethyl-2-pyridinyl)methyl]amino]ethyl][(3-ethyl-2-pyridinyl)methyl]amino]- (9CI) (CA INDEX NAME)



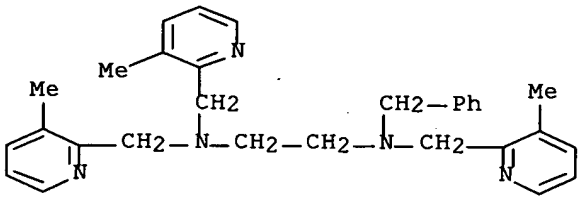
IT ***260395-26-4P 260395-27-5P 260395-28-6P 302542-62-7P***
RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)
(ligand; composition containing transition metal complex for catalytically bleaching laundry fabrics with atmospheric oxygen)
RN 260395-26-4 HCAPLUS
CN 1,2-Ethanediamine, N-methyl-N,N',N'-tris[(3-methyl-2-pyridinyl)methyl]- (9CI) (CA INDEX NAME)



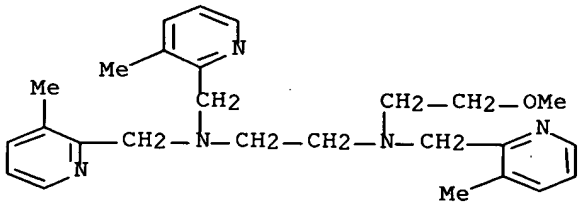
RN 260395-27-5 HCAPLUS
CN 1,2-Ethanediamine, N-ethyl-N,N',N'-tris[(3-methyl-2-pyridinyl)methyl]- (9CI) (CA INDEX NAME)



RN 260395-28-6 HCAPLUS
CN 1,2-Ethanediamine, N,N,N'-tris[(3-methyl-2-pyridinyl)methyl]-N'-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 302542-62-7 HCAPLUS
CN 1,2-Ethanediamine, N-(2-methoxyethyl)-N,N',N'-tris[(3-methyl-2-pyridinyl)methyl]- (9CI) (CA INDEX NAME)



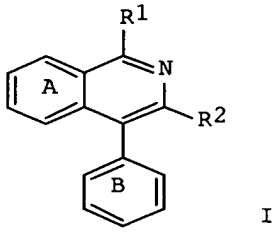
REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 25 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:712977 HCAPLUS Full-text
DOCUMENT NUMBER: 133:281699
TITLE: Preparation of isoquinoline derivatives as phosphodiesterase V inhibitors
INVENTOR(S): Ukita, Shinzo; Yamada, Koichiro; Ohmori, Kenji; Yoshikawa, Kohei
PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 49 pp.
CODEN: JKXXAF

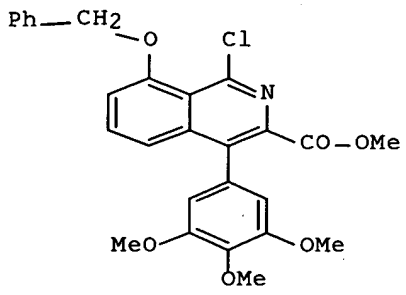
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000281654	A2	20001010	JP 1999-83022	19990326

PRIORITY APPLN. INFO.: JP 1999-83022 19990326
OTHER SOURCE(S): MARPAT 133:281699
GI



I



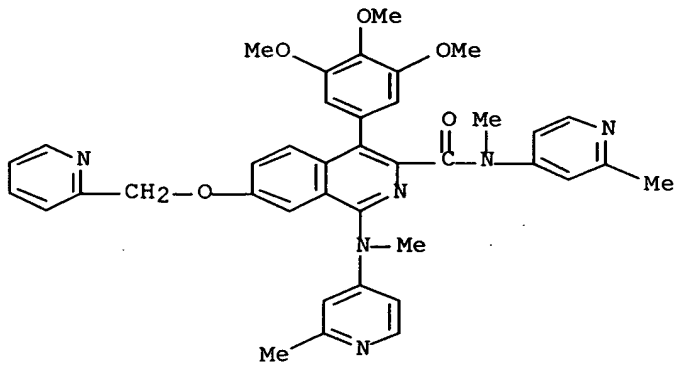
II

AB The title compds. I [ring A = benzene ring with substituents; ring B = (un)substituted benzene ring; R1 = (un)substituted alkoxy, halo, etc.; R2 = CO2R3, etc.; R3 = H, etc.], useful as phosphodiesterase V inhibitors (no data) for the treatment of circulatory system diseases (no data), are prepared For example, the title compound II was prepared

IT ***299170-44-8P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of isoquinoline derivs. as phosphodiesterase V inhibitors)

RN 299170-44-8 HCAPLUS

CN 3-Isoquinolinecarboxamide, N-methyl-1-[methyl(2-methyl-4-pyridinyl)amino]-N-(2-methyl-4-pyridinyl)-7-(2-pyridinylmethoxy)-4-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)



L36 ANSWER 26 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:335516 HCAPLUS Full-text
DOCUMENT NUMBER: 132:336136
TITLE: Detergent bleaching composition for bleaching/cleaning of fabrics
INVENTOR(S): Delroisse, Michel Gilbert Jose; Feringa, Bernard Lucas; Hage, Ronald; Hermant, Roelant Mathijs; Kalmeijer, Robertus Everardus; Koek, Jean Hypolites; Lamers, Christiaan; Rispens, Minze; Russell, Stephen William; Van Vliet, Ronaldus Theodorus Leonardus; Whittaker, Jane
PATENT ASSIGNEE(S): Unilever Plc, UK; Unilever Nv; Hindustan Lever Limited
SOURCE: PCT Int. Appl., 38 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

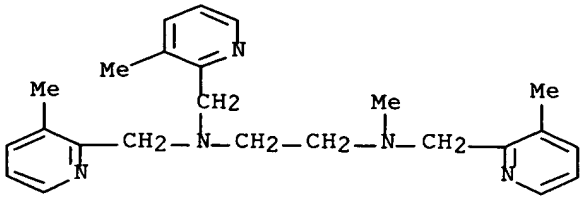
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000027975	A1	20000518	WO 1999-EP8324	19991025
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1008645	A1	20000614	EP 1998-309168	19981110
EP 1008645	B1	20040721		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
ES 2223108	T3	20050216	ES 1998-309168	19981110
CA 2350570	AA	20000518	CA 1999-2350570	19991025
BR 9915192	A	20010814	BR 1999-15192	19991025
AU 749526	B2	20020627	AU 2000-13780	19991025
IN 194492	A	20041113	IN 1999-BO749	19991102
US 6165963	A	20001226	US 1999-433156	19991103
PRIORITY APPLN. INFO.:			EP 1998-309168 A	19981110
			WO 1999-EP8324 A	19991025

OTHER SOURCE(S): MARPAT 132:336136

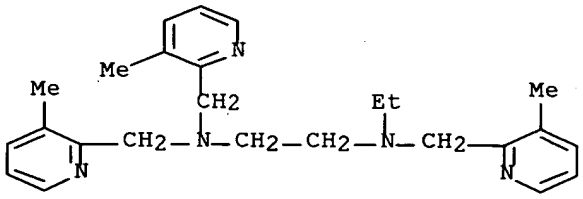
AB A detergent bleaching catalyst comprises a compound including a specified pentadentate N-containing ligand. The compound can activate H2O2 or peroxyacids and provides favorable stain removal properties, particularly in the presence of Fe, Mn or Cu ions. An improved stability in alkaline aqueous environment was obtained, in particular at the peroxy compound concns. generally present in the fabric washing liquor.

IT ***260395-26-4P 260395-27-5P 260395-28-6P 260395-29-7P***
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(ligand; metal complex bleach and oxidation catalysts for detergent)

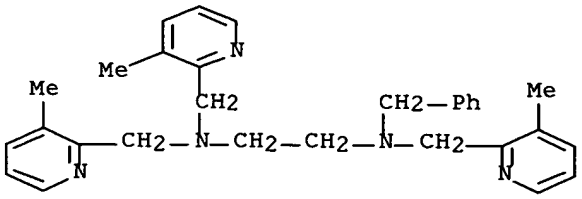
RN 260395-26-4 HCAPLUS
CN 1,2-Ethanediamine, N-methyl-N,N',N'-tris[(3-methyl-2-pyridinyl)methyl]- (9CI) (CA INDEX NAME)



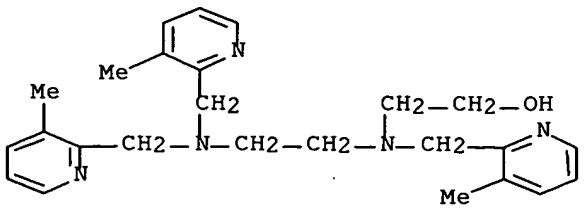
RN 260395-27-5 HCAPLUS
CN 1,2-Ethanediamine, N-ethyl-N,N',N'-tris[(3-methyl-2-pyridinyl)methyl]- (9CI) (CA INDEX NAME)



RN 260395-28-6 HCAPLUS
CN 1,2-Ethanediamine, N,N,N'-tris[(3-methyl-2-pyridinyl)methyl]-N'- (phenylmethyl)- (9CI) (CA INDEX NAME)



RN 260395-29-7 HCAPLUS
CN Ethanol, 2-[[2-[bis[(3-methyl-2-pyridinyl)methyl]amino]ethyl][(3-methyl-2-pyridinyl)methyl]amino]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 27 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:335113 HCAPLUS Full-text
DOCUMENT NUMBER: 132:323323
TITLE: Metal complex bleach and oxidation catalysts
INVENTOR(S): Delroisse, Michel Gilbert Jose; Hage, Ronald; Kalmeijer, Robertus Everardus; Lamers, Christiaan; Russell, Stephen William; Whittaker, Jane; Feringa, Bernard Lucas; Hermant, Roelant Mathijs; Koek, Jean Hypolites; Rispens, Minze Theunis; Van Vliet, Ronaldus Theodorus Leonardus
PATENT ASSIGNEE(S): Unilever PLC, UK; Unilever N.V.
SOURCE: Eur. Pat. Appl., 20 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1001009	A1	20000517	EP 1998-309169	19981110
EP 1001009	B1	20030903		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
ES 2206853	T3	20040516	ES 1998-309169	19981110
CA 2350571	AA	20000518	CA 1999-2350571	19991025
WO 2000027976	A1	20000518	WO 1999-EP8325	19991025
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
BR 9915193	A	20010814	BR 1999-15193	19991025
EP 1129170	A1	20010905	EP 1999-955934	19991025
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
TR 200101313	T2	20011022	TR 2001-200101313	19991025
AU 749674	B2	20020704	AU 2000-12682	19991025
US 6140294	A	20001031	US 1999-433157	19991103
PRIORITY APPLN. INFO.:			EP 1998-309169 A	19981110

WO 1999-EP8325 W 19991025

OTHER SOURCE(S): MARPAT 132:323323

AB A bleach and oxidation catalyst is provided comprising a catalytically active iron, manganese or copper complex including a specified pentadentate nitrogen-containing ligand. The metal complex can activate hydrogen peroxide or peroxyacids and provides favorable stain removal properties. In addition, a considerably improved stability of these metal complex compds. in alkaline aqueous environment has been obtained, in particular at the peroxy compound concns. generally present in the fabric washing liquor.

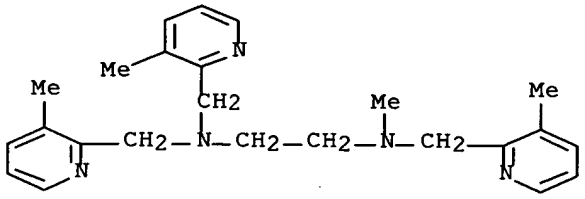
IT ***260395-26-4P 260395-27-5P 260395-28-6P 260395-29-7P***

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(ligand; metal complex bleach and oxidation catalysts)

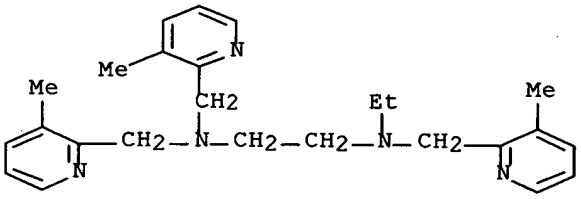
RN 260395-26-4 HCAPLUS

CN 1,2-Ethanediamine, N-methyl-N,N',N'-tris[(3-methyl-2-pyridinyl)methyl]- (9CI) (CA INDEX NAME)



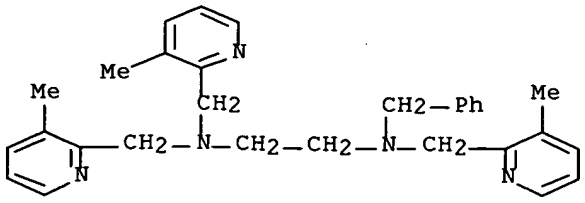
RN 260395-27-5 HCAPLUS

CN 1,2-Ethanediamine, N-ethyl-N,N',N'-tris[(3-methyl-2-pyridinyl)methyl]- (9CI) (CA INDEX NAME)

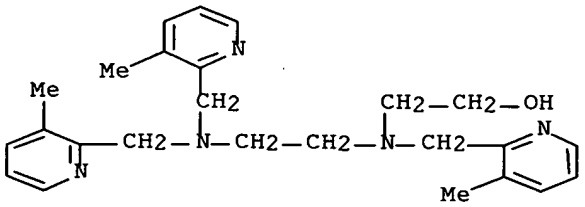


RN 260395-28-6 HCAPLUS

CN 1,2-Ethanediamine, N,N,N'-tris[(3-methyl-2-pyridinyl)methyl]-N'-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 260395-29-7 HCAPLUS
CN Ethanol, 2-[[2-[bis[(3-methyl-2-pyridinyl)methyl]amino]ethyl][(3-methyl-2-pyridinyl)methyl]amino]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 28 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:161523 HCAPLUS Full-text
DOCUMENT NUMBER: 132:209505
TITLE: Bleaching fabrics by atmospheric oxygen in the presence of transition metal complex catalysts
INVENTOR(S): Appel, Adrianus Cornelis Maria; Carina, Riccardo Filippo; Delroisse, Michel Gilbert Jose; Feringa, Bernard Lucas; Girerd, Jean-jacques; Hage, Ronald; Kalmeijer, Robertus Everardus; Martens, Constantinus Franciscus; Peelen, Jacobus Carolina Johannes; Que, Lawrence; Swarthoff, Ton; Tetard, David; Thornthwaite, David; Tiwari, Laxmikant; Thijssen, Rob; Twisker, Robin Stefan; Veerman, Simon Marinus; Van Der Voet, Gerrit; Smith, Richard George
PATENT ASSIGNEE(S): Unilever Plc, UK; Unilever Nv; Hindustan Lever Limited
SOURCE: PCT Int. Appl., 86 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 13
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000012808	A1	20000309	WO 1999-GB2878	19990901
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS,				

JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

CA	2342616	AA	20000309	CA 1999-2342616	19990901
AU	9956370	A1	20000321	AU 1999-56370	19990901
US	6245115	B1	20010612	US 1999-388171	19990901
EP	1109965	A1	20010627	EP 1999-943085	19990901
EP	1109965	B1	20050601		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO

TR	200101257	T2	20010821	TR 2001-200101257	19990901
BR	9913367	A	20020129	BR 1999-13367	19990901
EP	1433840	A1	20040630	EP 2004-7615	19990901

R: BE, DE, ES, FR, GB, IT

RU	2240391	C2	20041120	RU 2001-108575	19990901
AT	296915	E	20050615	AT 1999-943085	19990901
ES	2243071	T3	20051116	ES 1999-943085	19990901
CA	2364605	AA	20001012	CA 2000-2364605	20000322
WO	2000060043	A1	20001012	WO 2000-EP2587	20000322

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WO	2000060044	A1	20001012	WO 2000-EP2590	20000322

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TR	200102775	T2	20011221	TR 2001-2775	20000322
EP	1165738	A1	20020102	EP 2000-918830	20000322
EP	1165738	B1	20050727		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO

BR	2000009457	A	20020108	BR 2000-9457	20000322
AT	300604	E	20050815	AT 2000-918830	20000322
ES	2244424	T3	20051216	ES 2000-918830	20000322
US	6617299	B1	20030909	US 2000-539756	20000331
CA	2382114	AA	20010308	CA 2000-2382114	20000804
CA	2382115	AA	20010308	CA 2000-2382115	20000804
WO	2001016268	A1	20010308	WO 2000-EP7561	20000804

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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,

DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

WO 2001016269 A1 20010308 WO 2000-EP7563 20000804
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW
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BR 2000013592 A 20020507 BR 2000-13592 20000804

BR 2000013593 A 20020507 BR 2000-13593 20000804

EP 1208184 A1 20020529 EP 2000-951477 20000804
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL

EP 1208187 A1 20020529 EP 2000-960390 20000804
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL

TR 200200535 T2 20020722 TR 2002-535 20000804

AU 777434 B2 20041014 AU 2000-64400 20000804

CA 2383590 AA 20010308 CA 2000-2383590 20000816

CA 2383596 AA 20010308 CA 2000-2383596 20000816

CA 2383935 AA 20010308 CA 2000-2383935 20000816

WO 2001016270 A1 20010308 WO 2000-EP8075 20000816
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WO 2001016261 A2 20010308 WO 2000-EP8078 20000816

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BR 2000013744 A 20020514 BR 2000-13744 20000816

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	EP 1999-943083	A3 19990901
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	WO 2000-EP7561	W 20000804
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	WO 2000-EP8076	W 20000816
	WO 2000-EP8078	W 20000816
	US 2000-650134	A3 20000829

OTHER SOURCE(S): MARPAT 132:209505

AB Fabrics such as laundered fabrics are bleached by atmospheric O by treatment with transition metal complexes, that are applied in the dry form or in aqueous solns. (such as in laundering) or in nonaq. solns. (such in dry cleaning). The method can confer cleaning benefits to the textile after the treatment. A typical complex was manufactured by reaction of 2-pyridyl ketone oxime 1 h in EtOH-NH4OH containing NH4OAc with Zn at reflux, reaction of the resulting bis(pyridin-2-yl)methylamine 40 h with picolyl chloride hydrochloride in aqueous NaOH, reduction of the perchlorate salt of the 2nd intermediate with LiAlH4, lithiation of the 3rd intermediate with BuLi, methylation of 4th intermediate with MeI, and complexation of the resulting ligand with Fe(ClO4)2.6H2O.

IT ***260395-26-4P 260395-27-5P 260395-28-6P***

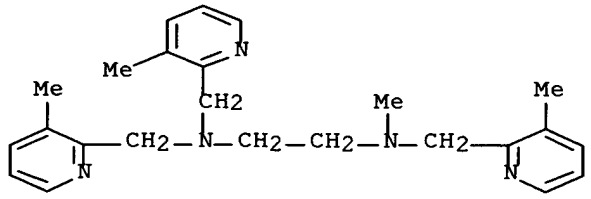
260395-29-7P

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(ligand; compns. containing transition metal complex catalysts for bleaching laundered fabrics with atmospheric oxygen)

RN 260395-26-4 HCAPLUS

CN 1,2-Ethanediamine, N-methyl-N,N',N'-tris[(3-methyl-2-pyridinyl)methyl]- (9CI) (CA INDEX NAME)



RN 260395-27-5 HCAPLUS

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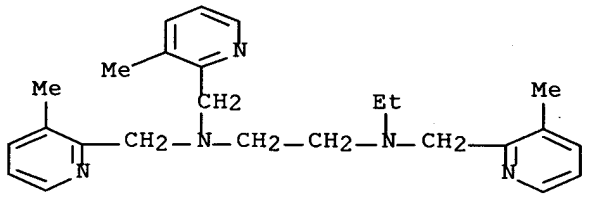

RN 260395-28-6 HCAPLUS

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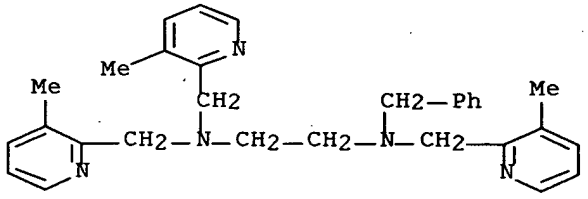

RN 260395-29-7 HCAPLUS

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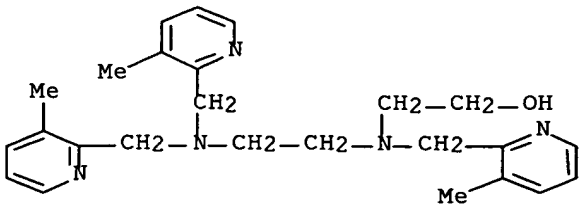

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 29 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:161417 HCAPLUS Full-text
DOCUMENT NUMBER: 132:209503
TITLE: Composition and method for bleaching a substrate such as laundered fabrics with atmospheric oxygen
INVENTOR(S): Appel, Adrianus Cornelis Maria; Carina, Riccardo Filippo; Delroisse, Michel Gilbert Jose; Feringa, Bernard Lucas; Girerd, Jean-jacques; Hage, Ronald; Kalmeijer, Robertus Everardus; Martens, Constantinus Franciscus; Peelen, Jacobus Carolina Johannes; Que, Lawrence; Swarthoff, Ton; Tetard, David; Thornthwaite, David; Tiwari, Laxmikant; Thijssen, Rob; Twisker, Robin Stefan; Veerman, Simon Marinus; Van Der Voet, Gerrit
PATENT ASSIGNEE(S): Unilever Plc, UK; Unilever Nv; Hindustan Lever Limited
SOURCE: PCT Int. Appl., 83 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 13
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000012667	A1	20000309	WO 1999-GB2876	19990901
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WO 2000-EP8078	W	20000816
WO 2000-EP8144	W	20000817
US 2000-650134	A3	20000829

OTHER SOURCE(S): MARPAT 132:209503

AB A method of bleaching a substrate such as laundered fabrics is provided that comprises applying to the substrate, in an aqueous medium, an transition metal complex, so that the complex catalyzes bleaching of the substrate by atmospheric oxygen. A typical complex was manufactured by reaction of 2-pyridyl ketone oxime 1 h in EtOH-NH4OH containing NH4OAc with Zn at reflux, reaction of the resulting bis(pyridin-2-yl)methylamine 40 h with picolyl chloride hydrochloride in aqueous NaOH, reduction of the perchlorate salt of the 2nd intermediate with LiAlH4, lithiation of the 3rd intermediate with BuLi, methylation of 4th intermediate with MeI, and complexation of the resulting ligand with Fe(ClO4)2.6H2O.

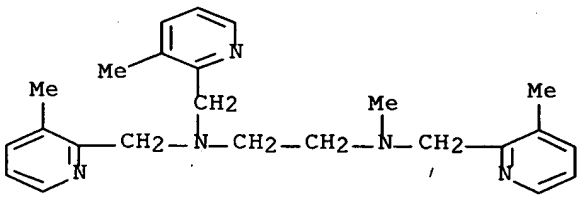
IT ***260395-26-4P 260395-27-5P 260395-28-6P 260395-29-7P***

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(ligand; compns. containing transition metal complex catalysts for bleaching laundered fabrics with atmospheric oxygen)

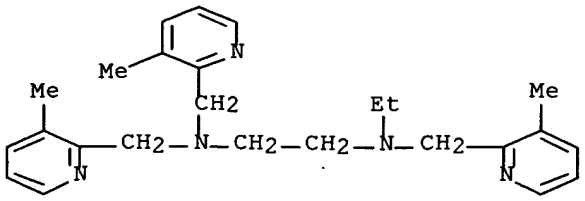
RN 260395-26-4 HCAPLUS

CN 1,2-Ethanediamine, N-methyl-N,N',N'-tris[(3-methyl-2-pyridinyl)methyl]-(9CI) (CA INDEX NAME)



RN 260395-27-5 HCAPLUS

CN 1,2-Ethanediamine, N-ethyl-N,N',N'-tris[(3-methyl-2-pyridinyl)methyl]-(9CI) (CA INDEX NAME)



RN 260395-28-6 HCAPLUS
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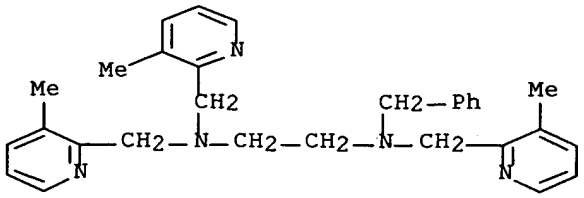

RN 260395-29-7 HCAPLUS
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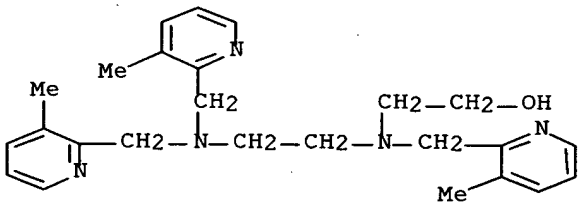


REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 30 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:66785 HCAPLUS Full-text
DOCUMENT NUMBER: 128:148788
TITLE: Raman Signature of the Fe2O2 "Diamond" Core
AUTHOR(S): Wilkinson, Elizabeth C.; Dong, Yanhong; Zang, Yan; Fujii, Hiroshi; Fraczkiewicz, Robert; Fraczkiewicz, Grazyna; Czernuszewicz, Roman S.; Que, Lawrence, Jr.
CORPORATE SOURCE: Department of Chemistry, University of Minnesota, Minneapolis, MN, 55455, USA
SOURCE: Journal of the American Chemical Society (1998),

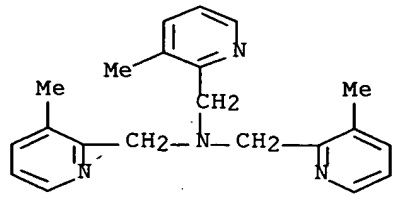
120(5), 955-962
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The authors report the resonance Raman (RR) spectra of iron complexes containing the Fe2(μ-O)2 core. Frozen CH3CN solns. of the FeIIIFeIV intermediate [Fe2(μ-O)2L2](ClO4)3 [L = TPA, 5-Me3-TPA, 5-Me2-TPA, 5-MeTPA, 5-Et3-TPA, or 3-Me3-TPA; TPA = tris(2-pyridylmethyl)amine] show numerous resonance-enhanced vibrations, and among these, an oxygen-isotope-sensitive vibration around 667 cm-1 that shifts .apprx.30 cm-1 when the samples are allowed to exchange with 18OH2, and whose Raman shift does not vary with Me substitution of the TPA ligand. Spectra of iron-isotope-substituted samples of [Fe2(μ-O)2(L)2](ClO4)3 (54Fe and 57Fe for L = TPA, and 54Fe and 58Fe for L = 5-Me3-TPA) show that this vibration is also iron-isotope-sensitive. These isotopic data taken together strongly suggest that this vibration involves motion of the Fe2(μ-O)2 core that is isolated from motions of the ligand. A frozen CH3CN solution of the diiron(III) complex [Fe2(μ-O)2(6-Me3-TPA)2](ClO4)2 (6-Me3-TPA = tris[(6-methyl-2-pyridyl)methyl]amine) shows one intense resonance-enhanced vibration at 692 cm-1 that shifts -30 cm-1 with 18O labeling. Normal coordinate anal. of the Fe2(μ-O)2 core in [Fe2(μ-O)2(5-Me3-TPA)2](ClO4)3 supports the assignment of the Fermi doublet centered around 666.2 cm-1 in the former and the peak at 692 cm-1 in the latter as a sym. vibration of this core. Also, the authors propose that this unique feature found at 650-700 cm-1 is indicative of a diamond core structure and is the Raman signature of an iron cluster containing this core.

IT ***202192-54-9P***, Tris(3-methyl-2-pyridylmethyl)amine
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for preparation of iron oxo-bridged tris(pyridylmethyl)amine dinuclear complex)

RN 202192-54-9 HCAPLUS

CN 2-Pyridinemethanamine, 3-methyl-N,N-bis[(3-methyl-2-pyridinyl)methyl]- (9CI) (CA INDEX NAME)



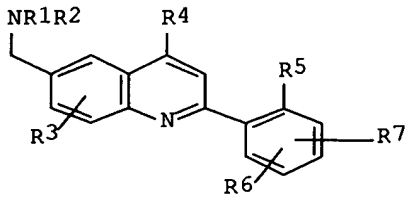
REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 31 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:22613 HCAPLUS Full-text
DOCUMENT NUMBER: 124:55811
TITLE: Preparation of quinoline derivatives as angiotensin II antagonists
INVENTOR(S): O. Josho; Okazoe, Takashi; Morisawa, Yoshitomi; Inoe,

Yoshihisa; Nakamura, Norifumi
PATENT ASSIGNEE(S): Asahi Glass Co Ltd, Japan; Green Cross Corp
SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07238071	A2	19950912	JP 1994-28247	19940225
PRIORITY APPLN. INFO.:			JP 1994-28247	19940225

OTHER SOURCE(S): MARPAT 124:55811
GI



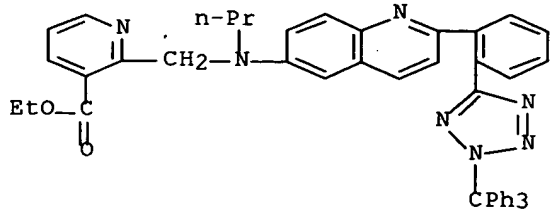
I

AB The title compds. I [R1, R2 = H, alkyl, etc.; R3 = H, halo, etc.; R4 = H, halo, CONH2, etc.; R5 = CN, etc.; R6, R7 = H, alkyl, etc.] are prepared Et 2-[N-propyl-N-[2-[2-(1H-tetrazol-5-yl)phenyl]quinolin-6-yl]methylamino]nicotinate (II) was prepared in a multistep process starting with 5-methylisatin and 2-acetylbenzoic acid. In an in vitro test for angiotensin II antagonism, II showed IC50 < 10-6 M.

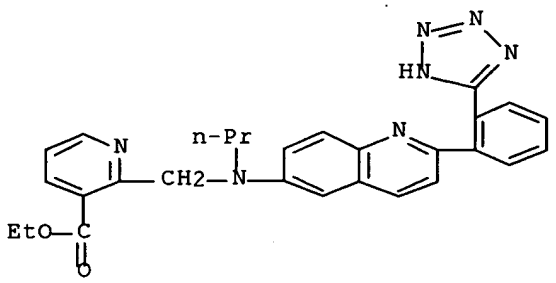
IT ***172210-98-9P 172210-99-0P 172211-00-6P***
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of quinoline derivs. as angiotensin II antagonists)

RN 172210-98-9 HCAPLUS

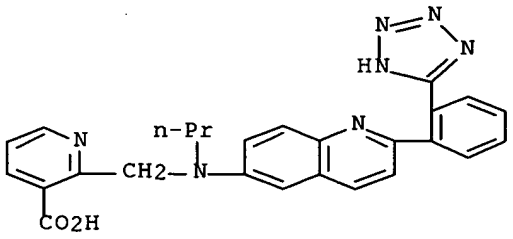
CN 3-Pyridinecarboxylic acid, 2-[[propyl[2-[2-[2-(triphenylmethyl)-2H-tetrazol-5-yl]phenyl]-6-quinolinyl]amino]methyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 172210-99-0 HCAPLUS
CN 3-Pyridinecarboxylic acid, 2-[[propyl[2-[2-(1H-tetrazol-5-yl)phenyl]-6-quinolinyl]amino]methyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 172211-00-6 HCAPLUS
CN 3-Pyridinecarboxylic acid, 2-[[propyl[2-[2-(1H-tetrazol-5-yl)phenyl]-6-quinolinyl]amino]methyl]- (9CI) (CA INDEX NAME)



L36 ANSWER 32 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:995855 HCAPLUS Full-text
DOCUMENT NUMBER: 124:145927
TITLE: Preparation of (aminoalkyl)quinoline or (aminoalkyl)quinazoline antiinflammatories and antiarthritics
INVENTOR(S): Sohda, Takashi; Makino, Haruhiko; Baba, Atsuo
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan
SOURCE: PCT Int. Appl., 95 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9524394	A1	19950914	WO 1995-JP330	19950302

W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, KG, KR, KZ, LK, LR, LT, LV, MD, MG, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TT, UA, US, UZ, VN

RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

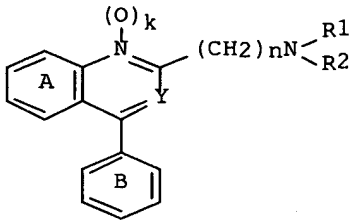
CA 2184392	AA	19950914	CA 1995-2184392	19950302
AU 9518609	A1	19950925	AU 1995-18609	19950302
EP 749426	A1	19961227	EP 1995-910723	19950302
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
TW 384285	B	20000311	TW 1995-84101956	19950302
JP 08225531	A2	19960903	JP 1995-47377	19950307
US 5650410	A	19970722	US 1995-416708	19950417

PRIORITY APPLN. INFO.:

JP 1994-36864	A	19940308
JP 1994-39476	A	19940310
JP 1994-316376	A	19941220
WO 1995-JP330	W	19950302

OTHER SOURCE(S): MARPAT 124:145927

GI



I

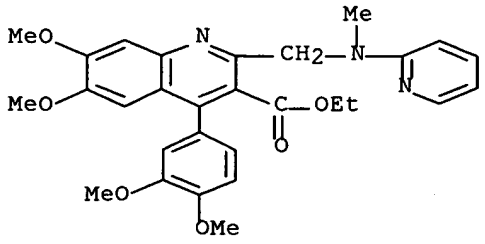
AB The title compds. [I; Y = N, CG; G = (un)esterified carboxyl group; R1, R2 = H, (un)substituted hydrocarbon, (un)substituted heterocyclyl, etc.; ring A and ring B may optionally be substituted; n = 1-4; k = 0, 1], useful as antiinflammatories and antiarthritics, are prepared Thus, Et2NH was condensed with Et 2-chloromethyl-4-(3,4-dimethoxyphenyl)-6,7- dimethoxyouinoline-3-carboxylate, producing Et 2-(N,N-diethylaminomethyl)- 4-(3,4-dimethoxyphenyl)-6,7-dimethoxyouinoline-3-carboxylate, m.p. 130-131°, which demonstrated a 103% edema inhibitory rate in a rat adjuvant arthritis model.

IT ***173253-29-7P***

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of (aminoalkyl)quinoline or (aminoalkyl)quinazoline antiinflammatories and antiarthritics)

RN 173253-29-7 HCAPLUS

CN 3-Quinolinecarboxylic acid, 4-(3,4-dimethoxyphenyl)-6,7-dimethoxy-2-[(methyl-2-pyridinylamino)methyl]-, ethyl ester (9CI) (CA INDEX NAME)



L36 ANSWER 33 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1993:147571 HCAPLUS Full-text
DOCUMENT NUMBER: 118:147571
TITLE: Preparation of N-(2-pyridinesulfonyl)-N'-(2-pyrimidinyl)urea derivatives as herbicides
INVENTOR(S): Sakashita, Nobuyuki; Nakajima, Toshio; Murai, Shigeo; Yoshida, Tsunezo; Nakamura, Yuji; Sawaki, Masahiko; Motosawa, Shoichi
PATENT ASSIGNEE(S): Ishihara Sangyo Kaisha, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 31 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04253974	A2	19920909	JP 1991-100628	19910205
PRIORITY APPLN. INFO.:			JP 1991-100628	19910205
OTHER SOURCE(S):	MARPAT 118:147571			

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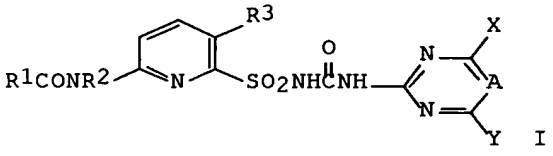
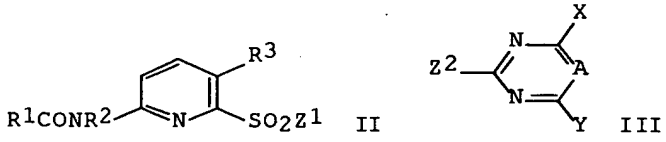


I



II III

AB The title compds. (I; R1 = cycloalkyl, alkoxyalkyl, (un)substituted Ph, pyridyl, thienyl, furyl, pyrazolyl, or piperazinyl; R2 = (halo)alkyl, cycloalkyl, Ph, PhCH2; R3 = H, halo, (halo)alkyl; X, Y = halo, alkyl, (halo) alkoxy; A = CH, N) are prepared by reaction of 2-pyridinesulfonamide derivs. (II; Z1 = NH2, isocyanato, NHCO2R4; R4 = alkyl, aryl; R1 - R3 = same as above)

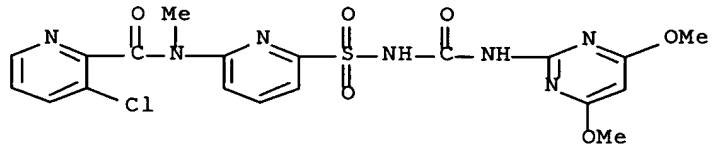
with pyrimidine derivs. (III; Z2 = NH2, when Z1 = isocyanato or NHCO2R4; Z2 = isocyanato or NHCO2R4, when Z1 = NH2). Thus, cyanation of 2,6-dibromopyridine with CuCN in refluxing DMF and hydrolysis of the resulting 2-bromo-6-cyanopyridine with aqueous NaOH followed by acidification gave 6-bromopicolinic acid. Chlorination of the latter compound with POCl3 under reflux, condensation of the product with N-tert-butyl-6-methylaminopyridine-2-ylsulfonamide in CH2Cl2 containing Et3N, and deprotection of the resulting 6-bromo-N-(6-tert- butylaminosulfonylpyridin-2-yl)-N-methylpicolinamide to 6-bromo-N-(6-aminosulfonylpyridin-2-yl)-N-methylpicolinamide followed by carbamoylation with Ph 2,4- dimethoxypyrimidin-2-yl carbamate gave I (R1 = 6-bromo-2-pyridyl, R2 = Me, R3 = H, X = Y = OMe, A = CH) (IV). IV at 0.31 g/are postemergence completely controlled Ipomoea and Amaranthus retroflexus. A total of 82 I were prepared and were also effective for controlling Sida spinosa and Echinochloa crus-galli.

IT ***146371-79-1P 146371-80-4P 146371-86-0P 146372-05-6P***

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as herbicide)

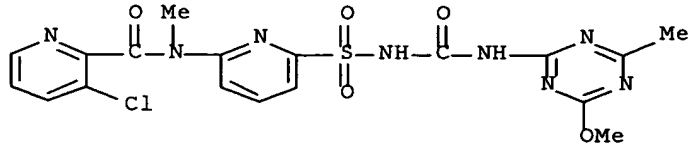
RN 146371-79-1 HCAPLUS

CN 2-Pyridinecarboxamide, 3-chloro-N-[6-[[[[(4,6-dimethoxy-2-pyrimidinyl)amino]carbonyl]amino]sulfonyl]-2-pyridinyl]-N-methyl- (9CI) (CA INDEX NAME)



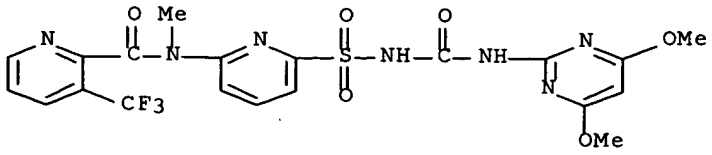
RN 146371-80-4 HCAPLUS

CN 2-Pyridinecarboxamide, 3-chloro-N-[6-[[[[(4-methoxy-6-methyl-1,3,5-triazin-2-yl)amino]carbonyl]amino]sulfonyl]-2-pyridinyl]-N-methyl- (9CI) (CA INDEX NAME)

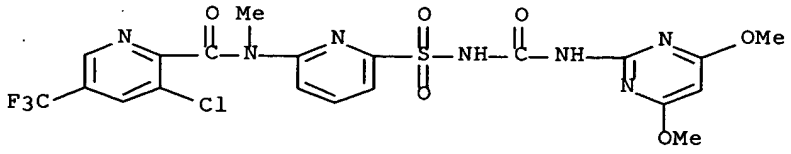


RN 146371-86-0 HCAPLUS

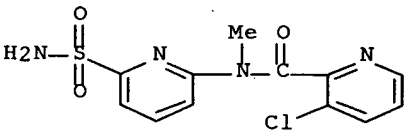
CN 2-Pyridinecarboxamide, N-[6-[[[[(4,6-dimethoxy-2-pyrimidinyl)amino]carbonyl]amino]sulfonyl]-2-pyridinyl]-N-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



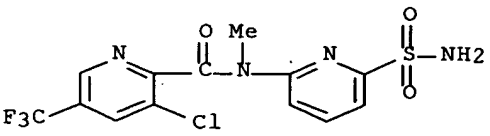
RN 146372-05-6 HCAPLUS
CN 2-Pyridinecarboxamide, 3-chloro-N-[6-[[[[(4,6-dimethoxy-2-pyrimidinyl)amino]carbonyl]amino]sulfonyl]-2-pyridinyl]-N-methyl-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)



IT ***146372-44-3P 146372-61-4P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for (pyridinesulfonyl)pyrimidinylurea herbicide)
RN 146372-44-3 HCAPLUS
CN 2-Pyridinecarboxamide, N-[6-(aminosulfonyl)-2-pyridinyl]-3-chloro-N-methyl- (9CI) (CA INDEX NAME)



RN 146372-61-4 HCAPLUS
CN 2-Pyridinecarboxamide, N-[6-(aminosulfonyl)-2-pyridinyl]-3-chloro-N-methyl-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L36 ANSWER 34 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1967:421848 HCAPLUS Full-text
DOCUMENT NUMBER: 67:21848
TITLE: New antitussive isoquinoline derivatives
PATENT ASSIGNEE(S): CIBA Ltd.
SOURCE: Fr. M., 10 pp.
CODEN: FMXXAJ
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 3782		19660131	FR	
BE 644126			BE	
CH 449013			CH	
FR 1389737			FR	
FR 1389738			FR	
GB 1021525			GB	
GB 1021526			GB	
US 3277085		19660000	US	
PRIORITY APPLN. INFO.:			CH	19630121
			CH	19640121

OTHER SOURCE(S): MARPAT 67:21848
GI For diagram(s), see printed CA Issue.
AB New antitussive isoquinoline derivs. with general formula (I) are prepared A mixture of 9 g. 1-chloro-3-chloromethyl-4-methylisoquinoline (II) and 40 cc. piperidine (III) is heated in a sealed tube 8 hrs. at 150°, the reaction mixture concentrated in vacuo, treated with water, and extracted with CH2Cl2, the extract dried and evaporated to dryness, and the residue in CHCl3 passed through activated alumina to give 4-methyl-1-piperidino-3-piperidinomethylisoquinoline, m. 111° (water-EtOH). The following products are prepared in a similar way (starting materials, reaction time, reaction temperature, final product, m.p., derivs., and m.p. given): II (9 g.), pyrrolidine (40 cc.), 8 hrs., 150°, 4-methyl-1-(1-pyrrolidinyl)-3- (1-pyrrolidinylmethyl)isoquinoline, -, hydrochloride, 239°; II (8 g.), N-methylpiperazine (IV) (50 cc.), 8 hrs., 150°, 4-methyl-1-(N'-methylpiperazino)-3-(N'-methylpiperazinomethyl)isoquinoline , 110-11°, hydrochloride, 238°; II (8 g.), N-(β-hydroxyethyl)piperazine (40 cc.), 8 hrs., 150°, 4-methyl-1-[N'-(β-hydroxyethyl)piperazino]-3-[N'-(β-hydroxyethyl)piperazinomethyl]isoquinoline, 112°, hydrochloride, 262° (decomposition); II (6 g.), Et2NH (15 cc.), 8 hrs., 150°, 4-methyl-1-diethylamino-3-diethylaminomethylisoquinoline, -, dimaleate, 109-11°; II (4.5 g.), ethanolamine (15 cc.), 3 hrs., 130°, 4-methyl-1-(β-hydroxyethylamino)-3-(β- hydroxyethylaminomethyl)isoquinoline, -, hydrochloride, 252-4°; II (5 g.), N-carbethoxypiperazine (V) (20 cc.), 6 hrs., 140°, 4-methyl-1-(N'-carbethoxypiperazino)-3-(N'-carbethoxypiperazinomethyl)isoq uinoline, 90-2°, -, -; II (5 g.), 2-methylpiperidine (20 cc.), 6 hrs., 140°, 1-chloro-4-methyl-3-(2-methylpiperidinomethyl)isoquinol ine (VI), 106-8°, -, -; VI (6 g.), morpholine (VII) (20 cc.), 14 hrs., 170°, 4-methyl-1-morpholino-3-(2-methylpiperidinomethyl)isoquinoline, 103-4°, -, -; 1-chloro-3-chloromethyl-4-methyl-5-nitroisoquinoline (VIII) (2 g.), VII (10 cc.), 2 hrs., 120°, 4-methyl-1-morpholino-3-morpholinomethyl-5- nitroisoquinoline (IX), 145-6°, -, -; VIII (2.5 g.), III (10 cc.), 2.5 hrs., 80°, 4-methyl-5-nitro-1-piperidino-3-

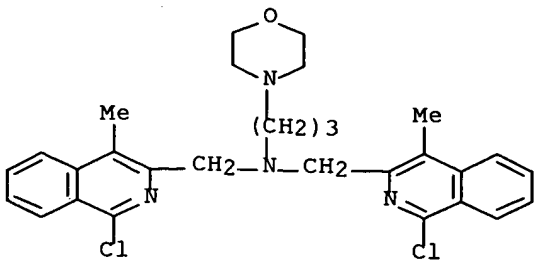
piperidinomethylisoquinoline, 104-6°, -, -; VIII (2.5 g.), p-anisidine (4.55 g.), EtOH (80 cc.), 4 hrs., reflux, 1-p-anisidino-3-p- anisidinomethyl-4-methyl-5-nitroisoquinoline, 183-5°, -, -; 1,7-dichloro-3-chloromethyl-4-methylisoquinoline (X) (4 g.), VII (50 cc.), 4 hrs., reflux, 7-chloro-4-methyl-1-morpholino-3- morpholinomethylisoquinoline, 120°, maleate, -; VIII (5 g.), III (8 cc.), EtOH (75 cc.), 1 hr., reflux, 1-chloro-4-methyl-5-nitro-3-piperidinomethylisoquinoline, 67-79°, -, -; II (4.5 g.), III (15 cc.), 2 hrs., 80°, 1-chloro-4-methyl-3- piperidinomethylisoquinoline, 79-80°, -, -; VIII (3.5 g.), IV (2.58 g.), EtOH (100 cc.), 2 hrs., reflux, 1-chloro-3-(N'-methylpiperazinomethyl)-4-methyl-5-nitroisoquinoline, 173-5°, -, -; VIII (4 g.), V (10 cc.), EtOH (75 cc.), 1 hr., reflux, 1-chloro-3-(N'-carbethoxypiperazinomethyl)-4-methyl-5-nitroisoquinoline, 127-8°, -, -; VIII (2.71 g.), diethanolamine (4.5 g.), dioxane (50 cc.), 3 hrs., reflux, 1-chloro-3-[bis(β-hydroxyethyl)aminomethyl]-4- methyl-5-nitroisoquinoline, 110-12°, -, -; II (5.0 g.), 4-methylpiperidine (5.5 cc.), 2 hrs., 80°, 1-chloro-3-(4- methylpiperidinomethyl)-4-methylisoquinoline, 83-5°, -, -; II (5.0 g.), concentrated aqueous NH3 (80 cc.), hydrated CuSO4 (1.0 g.), 30 hrs., 140°, bis(1-chloro-4-methyl-3-isoquinolylmethyl)amine, 131-2°, -, -; II (5.0 g.), N-(γ-aminopropyl)morpholine (6.5 g.), 2 hrs., 100°, N,N-bis(1-chloro-4-methyl-3-isoquinolylmethyl)-N- (γ-morpholinopropyl)amine, 110-12°, -, -. Some starting materials and other products are prepared as follows: II (6 g.) is added slowly with stirring to a cooled mixture of 15 cc. concentrated H2SO4 and 15 cc. fuming HNO3 and the mixture stirred 1.5 hrs. below 5° and poured over a mixture of ice and water to precipitate VIII, m 104-5° (EtOH). A mixture of 4 g. IX, 0.3 g. Pd-C and 150 cc. 95% EtOH is hydrogenated 1.5 hrs. to give 5-amino-4-methyl-1-morpholino-3-morpholinomethylisoquinoline (XI), m. 134-5° (EtOH). A solution of 1.6 g. NaNO2 in 5 cc. water is added slowly to a cooled solution of 8 g. XI in 6 cc. concentrated HCl and 6 cc. water, the resulting solution poured into a cooled solution of Cu2Cl2 (prepared from 8 g. CuSO4) and then is heated at 60°, and the precipitate suspended in 25 cc. water, alkalinized, and extracted with CHCl3 to give 5-chloro-4-methyl-1- morpholino-3-morpholinomethylisoquinoline, m. 104°. 4,4-Dimethylhomophthalimide (15 g.) is added slowly with stirring to a cooled (-10°) mixture of 30 cc. concentrated H2SO4 and 30 cc. fuming HNO3 and the mixture stirred 1 hr. below 20° and poured over a mixture of ice and water to precipitate 4,4-dimethyl-7-nitrohomophthalimide (XII), m. 209-11° (EtOH). A mixture of 23.4 g. XII, 0.5 g. Pd-C, and 200 cc. MeOH is hydrogenated at 50°/3.4 atmospheric .apprx.1.5 hrs. to give 4,4-dimethyl-7-aminohomophthalimide (XIII), m. 176-9° (MeOH). Concentrated H2SO4 (26 g.) is added slowly to a mixture of 20 g. XIII and 90 cc. water, and cooled at 0°, 8.4 g. NaNO2 in 24 cc. water added slowly to it, and this mixture is added slowly to a solution of Cu2Cl2 (prepared from 33.4 g. CuSO4), and the mixture heated at 60° 30 min., cooled, diluted with water, and extracted with CHCl3 to give 4,4-dimethyl-7- chlorohomophthalimide (XIV), m. 200° (EtOH). A mixture of 10 g. XIV, 0.5 cc. water, and 40 cc. POCl3 is heated in a sealed tube at 200° 5 hrs. to give X, m. 135° (hexane-CHCl3). Some recipes for the preparation of pharmacol. compns. are also given.

IT ***14657-55-7P***

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 14657-55-7 HCAPLUS

CN Isoquinoline, 3,3'-[[(3-morpholinopropyl)imino]dimethylene]bis[1-chloro-4-methyl- (8CI) (CA INDEX NAME)



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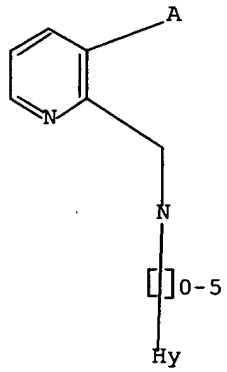

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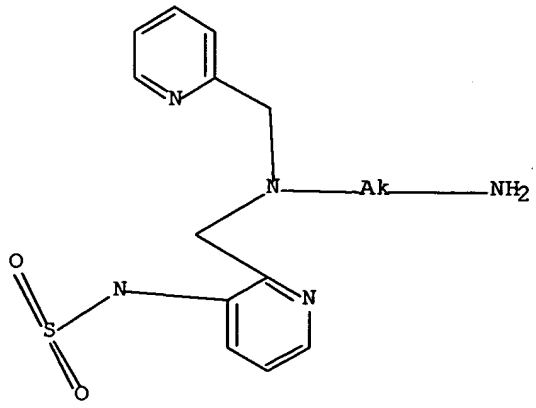

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Structure attributes must be viewed using STN Express query preparation.
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L9   ANSWER 1 OF 1  HCAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:         2004:878165  HCAPLUS  Full-text
DOCUMENT NUMBER:          141:379809
TITLE:                    Preparation of pyridine derivatives as CXCR4 chemokine
                          receptor binding compounds
INVENTOR(S):              Bridger, Gary; McEachern, Ernest J.; Skerlj, Renato;
                          Schols, Dominique
PATENT ASSIGNEE(S):       USA
SOURCE:                   U.S. Pat. Appl. Publ., 211 pp.
                          CODEN: USXXCO
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

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     US 2004209921         A1    20041021    US 2004-823494           20040412
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     WO 2004091518         A2    20041028    WO 2004-US11328          20040412
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OTHER SOURCE(S):          MARPAT 141:379809
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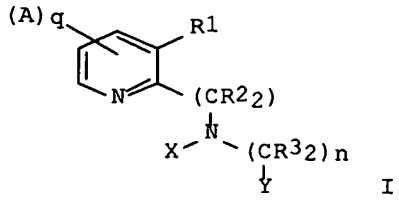

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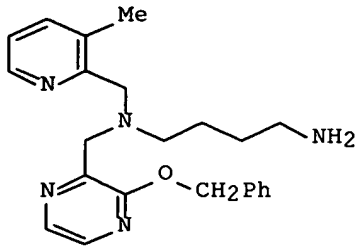


II

AB Title compds. I [X = (CR32)o-(CR3=CR3)p-(CR32)r-NR52, (CR32)s-R4, (un)substituted mono or bicyclic ring optionally containing N, O or S, etc.; Y = (un)substituted N-containing monocyclic or bicyclic aromatic or partially aromatic moiety; A and R1 = non-interfering substituent provided that two As do not form a ring; R2 and R3 = H or (un)substituted alkyl; R4 = (un)substituted heterocycle or a hetero compound; R5 = H or alkyl; wherein R1 and R2 is not H; and wherein R1 and R2 may be connected to form an addnl. ring if Y does not contain a 2-imidazoyl residue optionally connected to an addnl. ring; q and n independently = 0-4; p = 0-1; o and r independently = 1-4; s = 1-6 provided that if X = (CR3)2-R4, r is at least two if R4 = 2-pyridinyl, quinolinyl, imidazolyl or furan], as well as their pharmaceutically acceptable salts, are prepared and disclosed as having the ability to bind to chemokine receptors, in particular CXCR4. Thus, e.g., II was prepared by reductive amination of {4-[(3-methylpyridin-2-ylmethyl)-amino]- butyl}carbamic acid tert-Bu ester (preparation given) with 3-benzyloxypyrazine- 2-carbaldehyde. The present invention also relates to methods of using such compds., such as in treating HIV infection and inflammatory conditions such as rheumatoid arthritis. In assays to evaluate inhibition of HIV-1, many compds. of the invention exhibited IC50 values in the range of 0.5nM-5μM. Furthermore, the present invention relates to methods to elevate progenitor and stem cell counts, as well as methods to elevate white blood cell counts, using such compds.

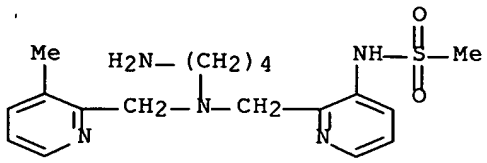
IT ***780796-24-9P***

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of pyridine derivs. as CXCR4 chemokine receptor binding compds.)

RN 780796-24-9 HCAPLUS

CN Methanesulfonamide, N-[2-[[(4-aminobutyl)[(3-methyl-2-pyridinyl)methyl]amino]methyl]-3-pyridinyl]-, tetrahydrobromide (9CI) (CA INDEX NAME)



●4 HBr

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FILE 'MARPAT' ENTERED AT 15:22:01 ON 17 OCT 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE CONTENT: 1961-PRESENT VOL 145 ISS 16 (20061013/ED)

SOME MARPAT RECORDS ARE DERIVED FROM INPI DATA FOR 1961-1987

MOST RECENT CITATIONS FOR PATENTS FROM MAJOR ISSUING AGENCIES
(COVERAGE TO THESE DATES IS NOT COMPLETE):

US	7108861	19 SEP 2006
DE	102005006940	24 AUG 2006
EP	1690960	16 AUG 2006
JP	2006222260	24 AUG 2006
WO	2006089024	24 AUG 2006
GB	2423085	16 AUG 2006
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CA	2492565	13 JUL 2006

Expanded G-group definition display now available.

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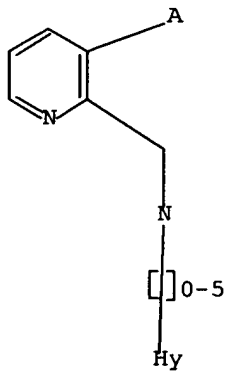

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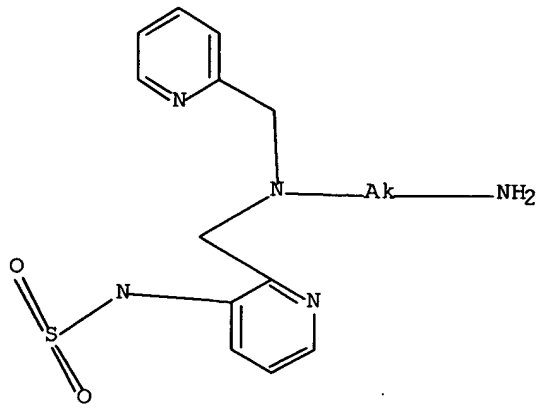

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L15 ANSWER 1 OF 3 MARPAT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 139:281335 MARPAT Full-text
TITLE: Technetium-dipyridine and other complexes as radiopharmaceuticals
INVENTOR(S): Babich, John W.; Maresca, Kevin P.
PATENT ASSIGNEE(S): Biostream, Inc., USA
SOURCE: PCT Int. Appl., 71 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003077727	A2	20030925	WO 2003-US7328	20030311
WO 2003077727	A3	20040902		

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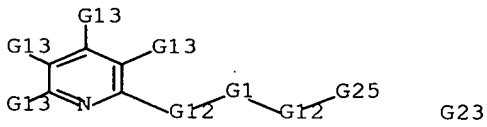
JP 2005519957	T2	20050707	JP 2003-575786	20030311
PRIORITY APPLN. INFO.:			US 2002-363142P	20020311
			WO 2003-US7328	20030311

AB One aspect of the invention relates to novel complexes of technetium (Tc) with various heteroarom. ligands, e.g., pyridyl and imidazolyl ligands, and their use in radiopharmaceuticals for a variety of clin. diagnostic and therapeutic applications. Another aspect of the invention relates to novel pyridyl ligands that form a portion of the aforementioned complexes. Methods for the preparation of the technetium complexes are also described. Another aspect of the invention relates to novel pyridyl ligands based on derivatized lysine, alanine and bis-amino acids for conjugation to small peptides by solid phase synthetic methods. Addnl., the invention relates to methods for imaging regions of a mammal using the complexes of the invention.

MSTR 1



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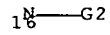

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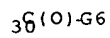

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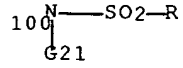

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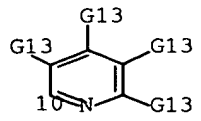

Patent location: claim 1
Note: or complexes with G23
Note: also incorporates claim 24

L15 ANSWER 2 OF 3 MARPAT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 137:232446 MARPAT Full-text
TITLE: Preparation of aminodicarboxylic acids for the treatment of cardiovascular diseases
INVENTOR(S): Alonso-Alija, Cristina; Haerter, Michael; Hahn, Michael; Pernerstorfer, Josef; Weigand, Stefan; Stasch, Johannes-Peter; Wunder, Frank
PATENT ASSIGNEE(S): Bayer Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 159 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002070510	A2	20020912	WO 2002-EP1891	20020222
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US 2004082798	A1	20040429	US 2003-469817	20031222
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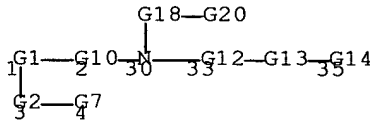
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [Z = saturated or partially unsatd. Ph, aromatic, heteroarom. containing 1-3 heteroatoms, e.g., S, N, O; V = absent, O, NR4, etc; Q = absent, (un)substituted alkylene, alkendiyl, etc.; Y = H, (un)substituted aryl, NR8R9, etc.; W = (un)substituted alkylene, alkendiyl; U = (un)substituted alkyl; A = (un)substituted aryl, heteroarom. containing 1-3 heteroatoms, e.g., S, N, O; X = (un)substituted alkylene, alkendiyl, aryl, etc.; R1 = tetrazolyl, COOR30, CONR31R32 ; R2 = tetrazolyl, COOR24, CONR25R26, R25 and R26 form 5 or 6-membered ring which can be interrupted by O or N; R3 = H, halo, (un)substituted alkyl, etc.; R4 = H, alkyl, cycloalkyl, etc.; R8, R9 = H, (un)substituted alkyl, alkenyl, etc; R24 = H, (un)substituted alkyl, cycloalkyl; R25, R26 = H, (un)substituted alkyl, cycloalkyl, etc.; R30 = H, (un)substituted alkyl, cycloalkyl; R31, R32 = H, (un)substituted alkyl, cycloalkyl,etc.; m = 1-4; n = 1-2] and their pharmaceutically acceptable salts were prepared For example, Pd(Ph3)2Cl2 mediated coupling of aryl bromide II, prepared from 3,4-bis(chloromethyl)- 2,5-dimethyl thiophene in 5-steps, with 2,4-dichlorophenyl boronic acid, followed by ester hydrolysis afforded aminodicarboxylate III. In vitro artery ring vasorelaxation activity of 7-examples of I are reported, with IC50 values ranging from 125-2 nM, e.g., aminodicarboxylate III IC50 = 2 nM. Compds. I stimulated the activation of soluble guanylate cyclase (sGC) independent of the heme group.

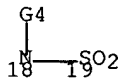
MSTR 1A



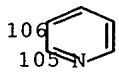
G1 = 204-2 205-3

G2 = 5-1 6-4

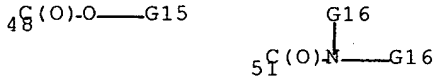
G5 = 18-1 19-6



G10 = C(O)
G12 = CH2
G13 = 105-33 106-35

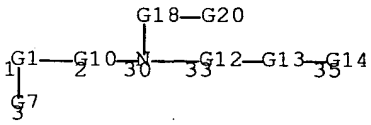


G18 = alkylene <containing 1-12 C>
(opt. substd. by 1 or more G19)
G20 = 48 / 51

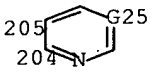


G25 = CH
Patent location: claim 1
Note: additional derivatization also claimed
Note: and salts
Stereochemistry: and stereoisomers

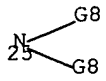
MSTR 1B



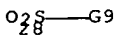
G1 = 204-2 205-3



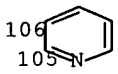
G7 = 25



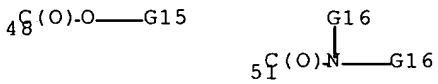
G8 = 28



G10 = C(O)
G12 = CH2
G13 = 105-33 106-35



G18 = alkylene <containing 1-12 C>
(opt. substd. by 1 or more G19)
G20 = 48 / 51



G25 = CH
Patent location: claim 1
Note: additional derivatization also claimed
Note: and salts
Stereochemistry: and stereoisomers

L15 ANSWER 3 OF 3 MARPAT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 120:107009 MARPAT Full-text
TITLE: 6-Amino-substituted imidazo[4,5-b]pyridine angiotensin II antagonists
INVENTOR(S): Greenlee, William J.; Kim, Dooseop; Mantlo, Nathan B.; Pastchett, Arthur A.; Rivero, Ralph A.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: U.S., 32 pp. Cont.-in-part of U.S. Ser. No. 516,286.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5223499	A	19930629	US 1992-881453	19920511
US 5332744	A	19940726	US 1990-516286	19900504
WO 9323399	A1	19931125	WO 1993-US4438	19930511
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RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9342437	A1	19931213	AU 1993-42437	19930511
EP 640084	A1	19950301	EP 1993-911232	19930511
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JP 07508028	T2	19950907	JP 1993-503696	19930511
FI 9403730	A	19940812	FI 1994-3730	19940812
FI 97471	B	19960913		
FI 97471	C	19961227		
PRIORITY APPLN. INFO.:			US 1989-358971	19890530
			US 1990-516286	19900504
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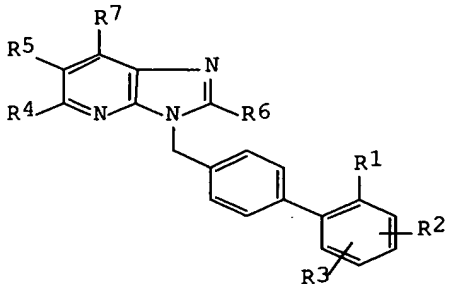
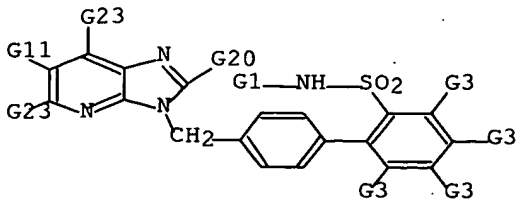


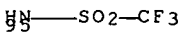
I

AB The title compds. I [R1 = (un)substituted SO2NHCOR23; R23 = aryl, heteroaryl, C3-6 cycloalkyl, (un)substituted NH2, etc.; R2, R3 = H, Cl, Br, iodo, F, (un)substituted C1-6 alkyl, (un)substituted C1-6 alkoxy, polyfluoro C1-4 alkyl, aryl, C1-6 alkoxyalkyl; R4, R7 = H, C1-5 alkyl, C1-5 polyfluoroalkyl, C3-6 cycloalkyl, Cl, Br, iodo, F, C1-5 alkoxy, etc.; R5 = (un)substituted NH2, morpholino, heterocyclyl, etc.; R6 = (un)substituted C1-9 alkyl, (un)substituted C2-6 alkenyl, (un)substituted C2-6 alkynyl, polyfluoro C1-4 alkyl, etc.], useful as angiotensin II receptor antagonists (no data), are prepared Thus, 2-butyl-3-[[2'-[[(3- cyclopentyl-1-oxopropyl)amino]sulfonyl][1,1'-biphenyl]-4-yl]methyl]-6-[(1- oxopentyl)amino]-3H-imidazo[4,5-b]pyridine was prepared from 2-amino-3-nitropyridine in 5 steps.

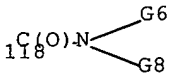
MSTR 1A



G6 = alkyl <containing 1-6 C> (opt. substd. by G7)
G7 = pyridyl
G8 = alkyl <containing 1-7 C> (opt. substd. by G9)
G9 = NH2
G11 = 95

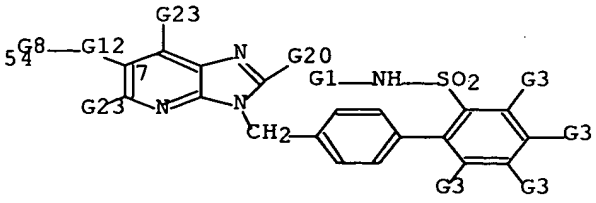


G23 = 118

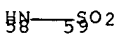


Derivative: or pharmaceutically acceptable salts
Patent location: claim 1

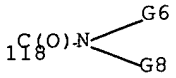
MSTR 1B



G6 = alkyl <containing 1-6 C> (opt. substd. by G7)
G7 = pyridyl
G8 = alkyl <containing 1-7 C> (opt. substd. by G9)
G9 = NH2
G12 = 58-7 59-54

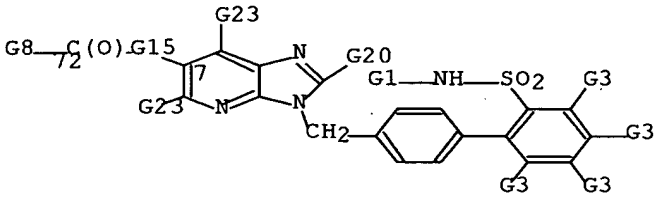


G23 = 118

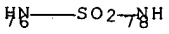


Derivative: or pharmaceutically acceptable salts
Patent location: claim 1

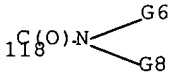
MSTR 1C



G6 = alkyl <containing 1-6 C> (opt. substd. by G7)
G7 = pyridyl
G8 = alkyl <containing 1-7 C> (opt. substd. by G9)
G9 = NH2
G15 = 76-7 78-72



G23 = 118



Derivative: or pharmaceutically acceptable salts
Patent location: claim 1